The Bethe-Salpeter Equation

Lucia Reining & Francesco Sottile
Palaiseau Theoretical Spectroscopy Group

The Bethe-Salpeter Equation

→ Concepts: embedding, auxiliary systems, s.c. functionals, Dyson eq.s

→ TD-GFT

→ The electron-hole problem

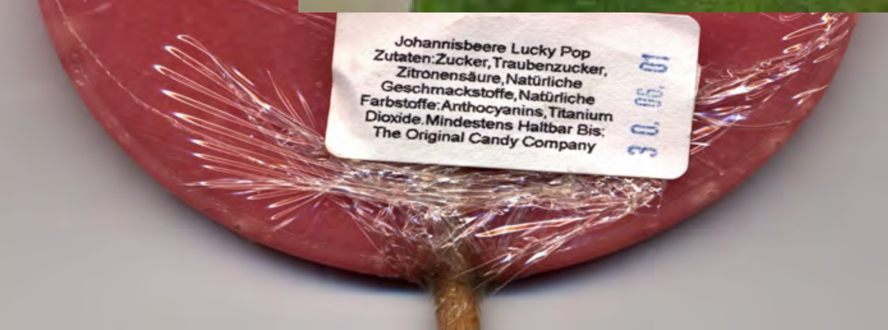
→ Approximations

→ Realizations

→ Applications

→ Notes

→ Theoretical Spectroscopy: aims and observations



Key quantities:

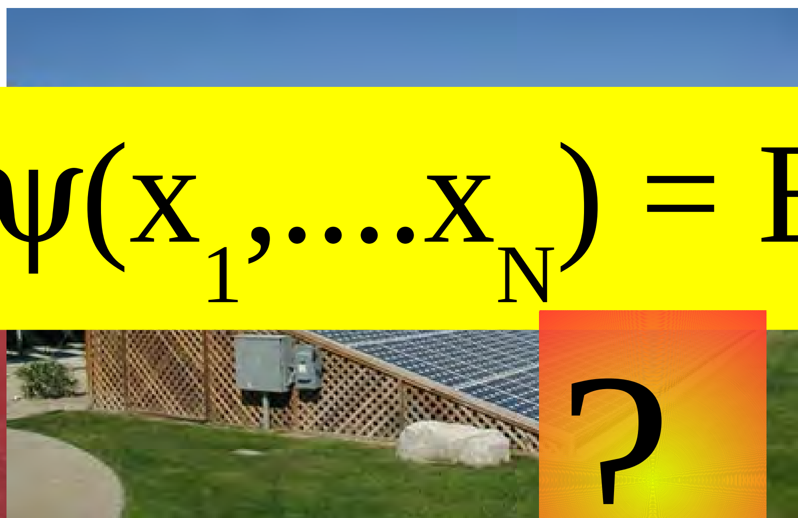
$$W(\omega) = \varepsilon^{-1}(\omega)\, v$$

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

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

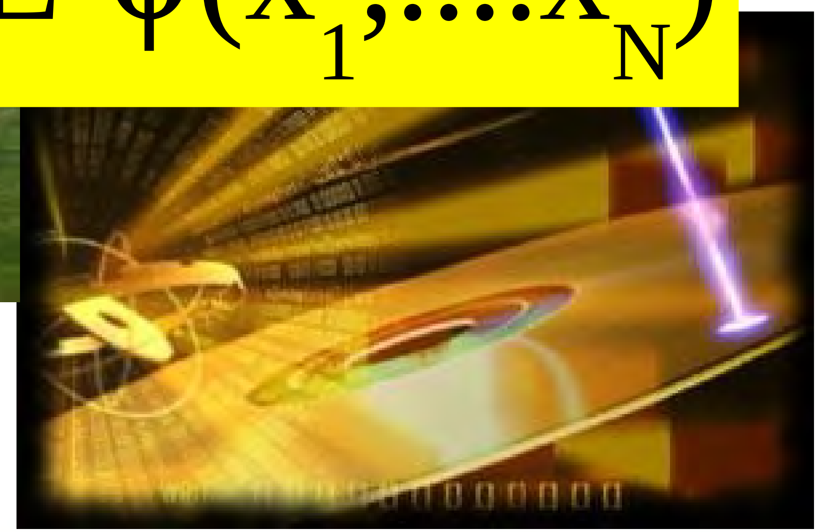
$$\delta n(\omega) = \chi(\omega)\, \delta V_{ext}(\omega)$$

→ Theoretical Spectroscopy: aims and observations



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

?



Embedding

What is the effective hamiltonian?

$$\begin{bmatrix} S & C_1 \\ C_2 & R \end{bmatrix} \times \begin{bmatrix} \phi_1 \\ \phi_2 \end{bmatrix} = \omega \begin{bmatrix} \phi_1 \\ \phi_2 \end{bmatrix} \tag{1}$$

$$\phi_2 = -(R - \omega)^{-1} C_2 \phi_1. \tag{2}$$

$$\left[S - C_1 (R - \omega)^{-1} C_2\right] \phi_1 \equiv \tilde{S}(\omega)\phi_1 = \omega \phi_1, \tag{3}$$

If one asks for a part of the solution, an effective ω-dependent hamiltonian appears.

(auxiliary system)

→ Concepts: $\phi \rightarrow O$

Observables can be simulated by an effective world

A practical example, simulate zero gravity

(expectation values)

→ Concepts: calculate only expectation values

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

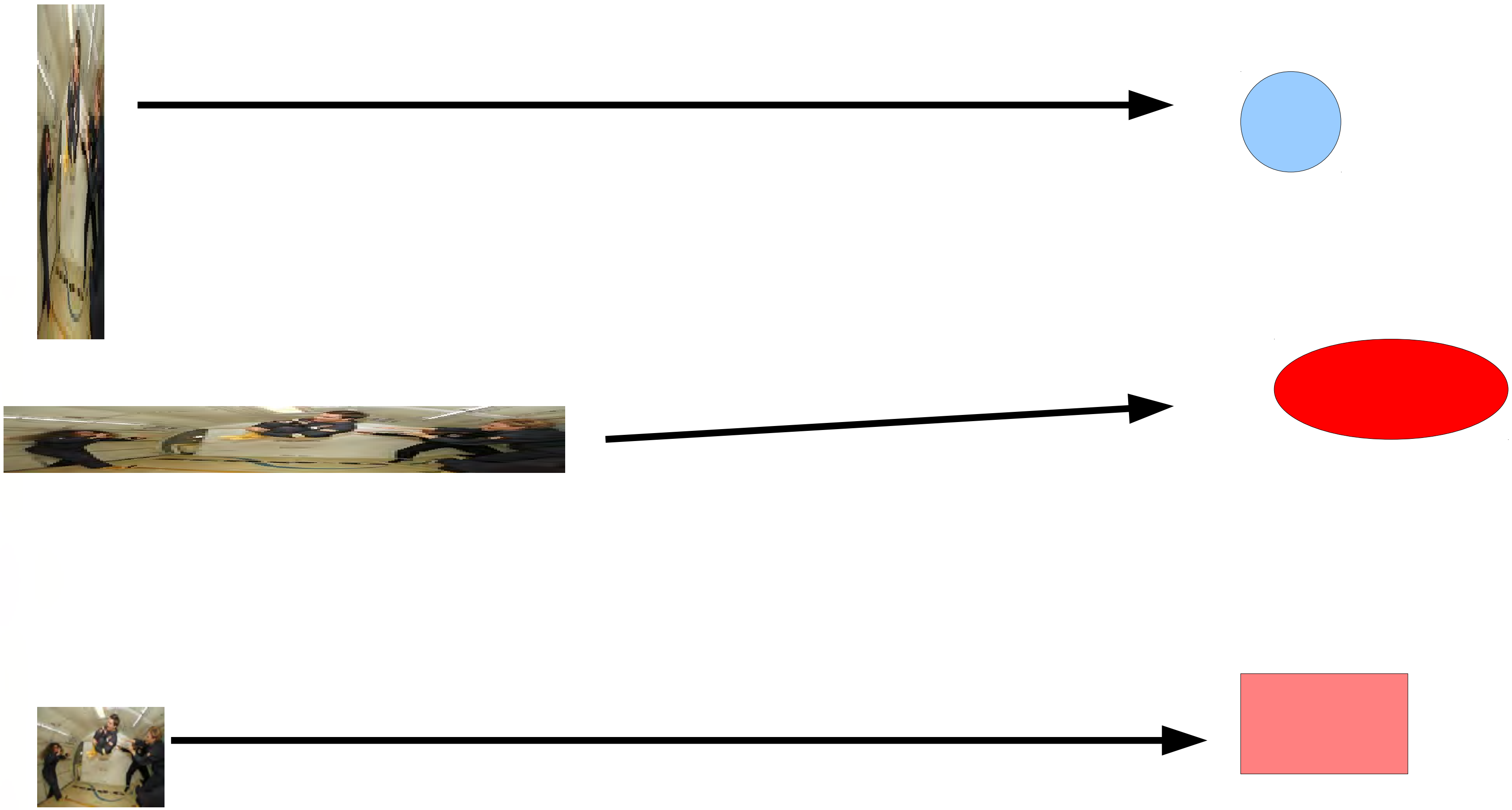
→ expectation values like

* density
* spectral functions
* dielectric function

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

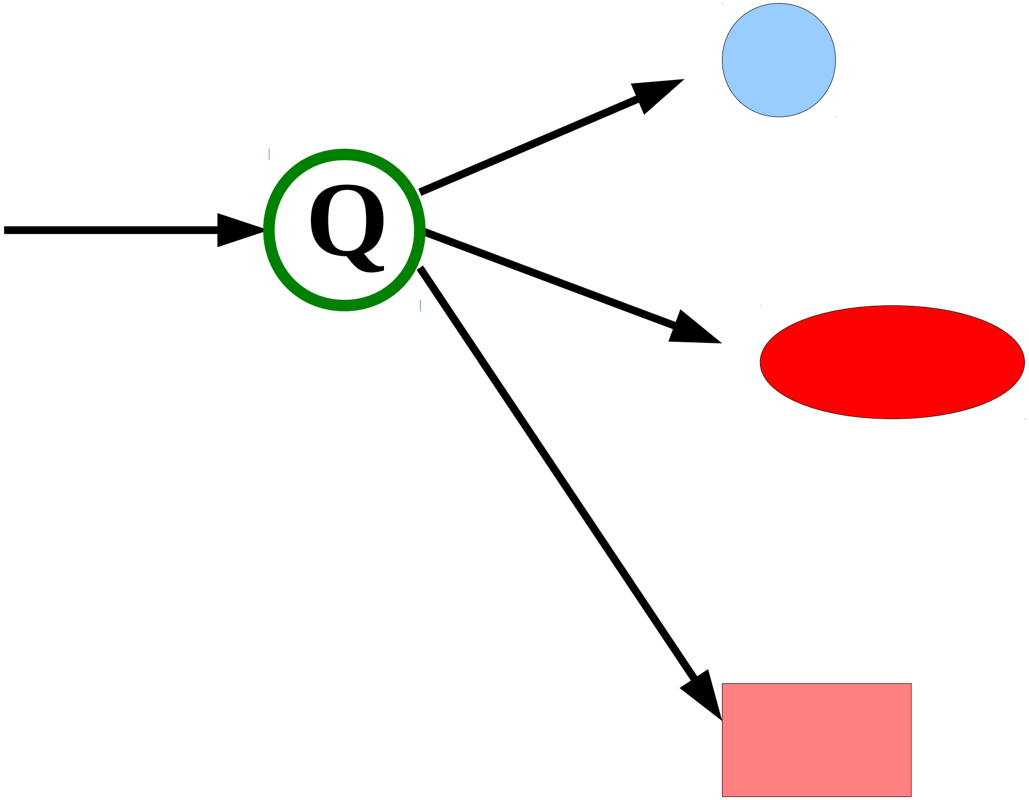
Do not want: → *all many-body* $\psi_n(x_1,....x_N)$

One effective world (auxiliary system) for every observable?



→ Concepts: $\phi \rightarrow Q$

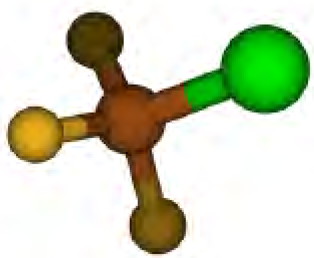
Use effective key quantities from which we get expectation values

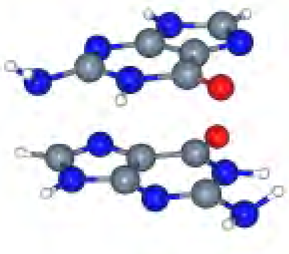


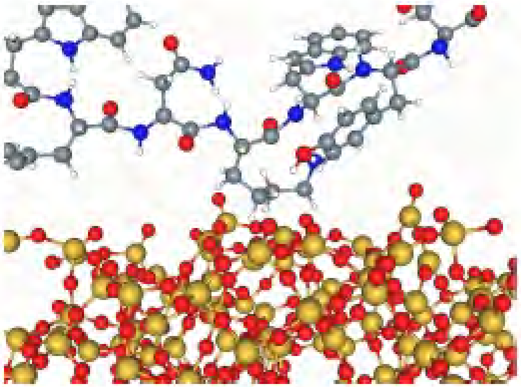
→ The effective quantities:

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

CI, QMC — GF methods (GW, BSE) — DF







Used to calculate expectation values

→ Illustration: DFT

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

LDA or so

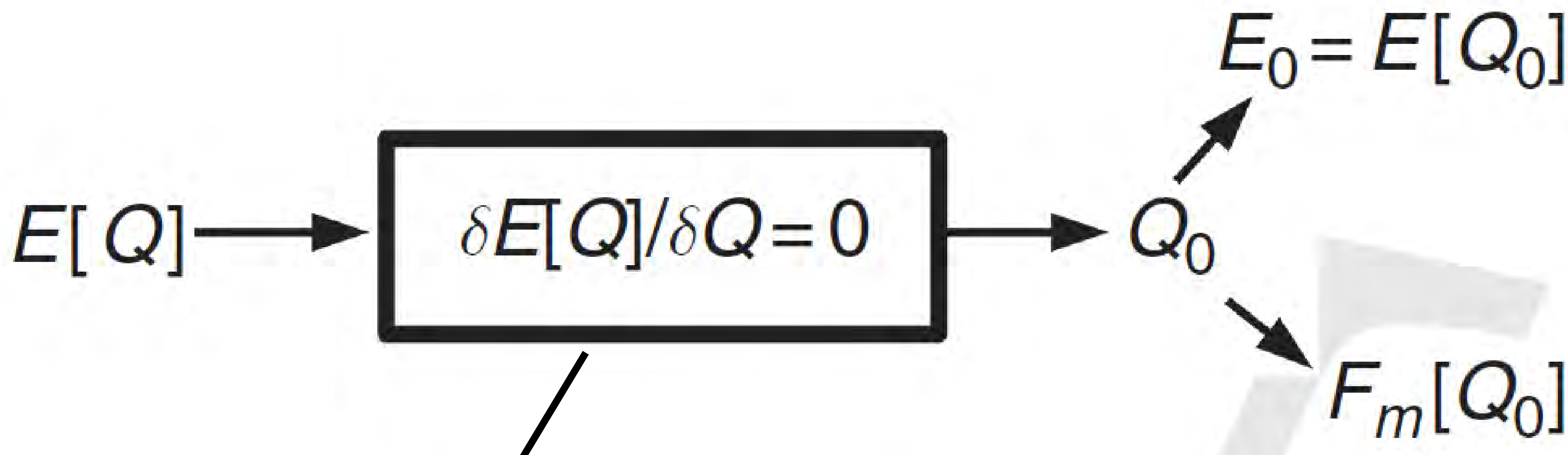
$$v_{\text{eff}}(\mathbf{r}) = \quad v_{\text{ext}}(\mathbf{r}) + v_{\text{H}}([n],\mathbf{r}) + v_{\text{xc}}([n],\mathbf{r})$$

Effective (auxiliary) world → Q = density

Direct access to density and top valence (independent-particle expression)

NOT to bandgaps, for example!!!

Hohenberg-Kohn-Sham



DFT: KS equation

$E[n] \rightarrow \delta E/\delta n = 0 \rightarrow n_0 \rightarrow E_0 = E[n_0]$

$\rightarrow F_0 = F[n_0]$???

Approximations needed for almost all observables!

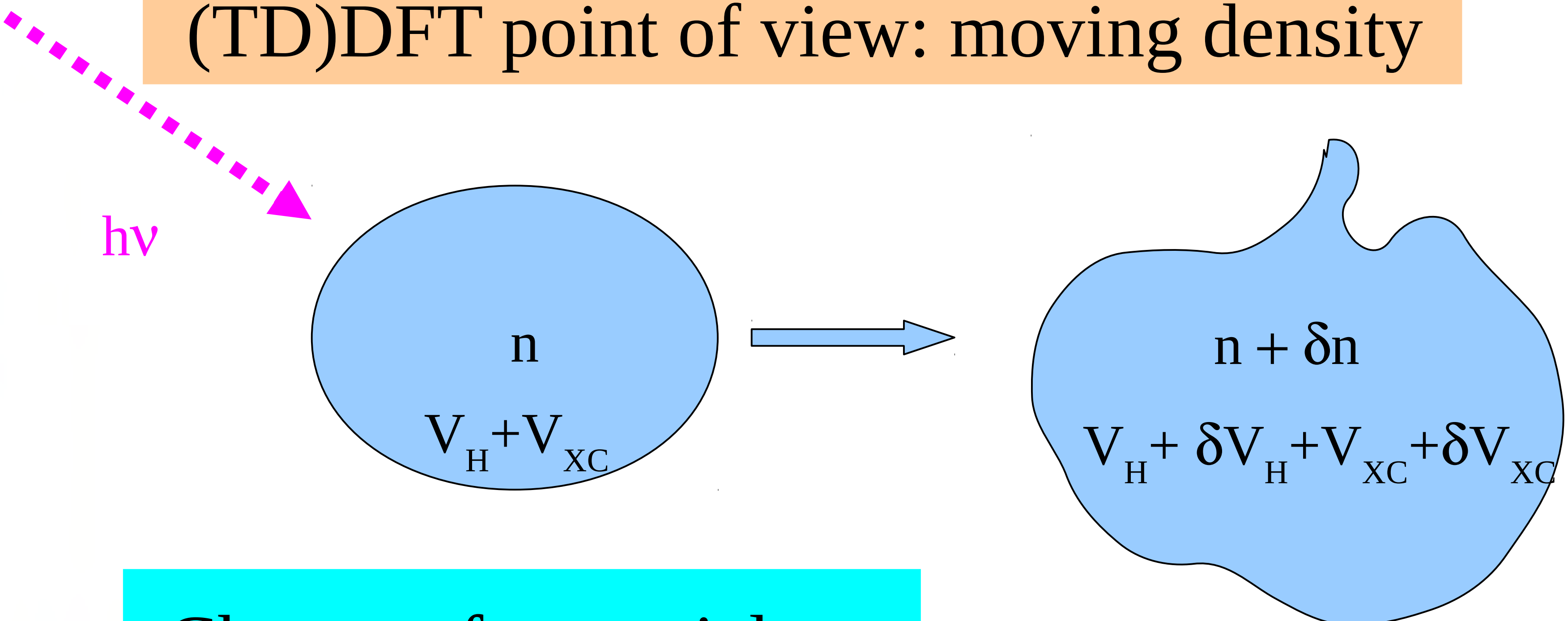
→ Response?

Effective quantities in an effective world

Time-dependent quantities – TD world

TDDFT intuitive :

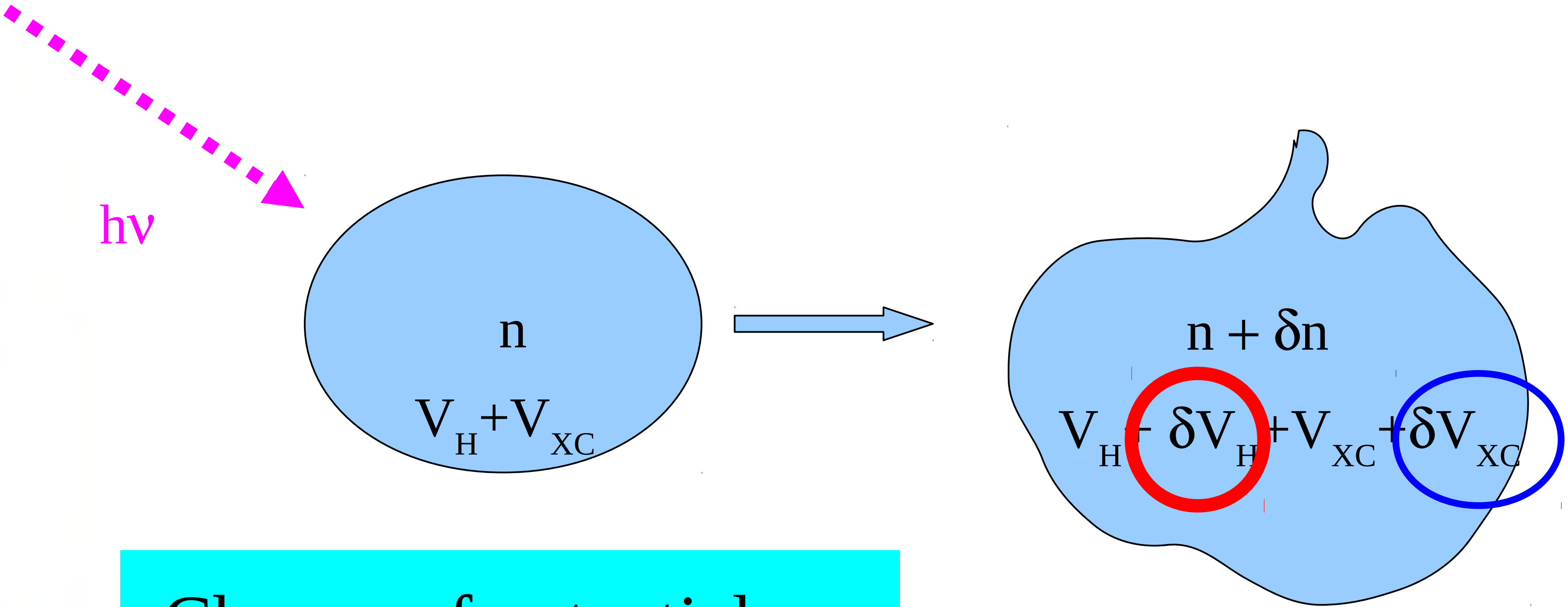
(TD)DFT point of view: moving density



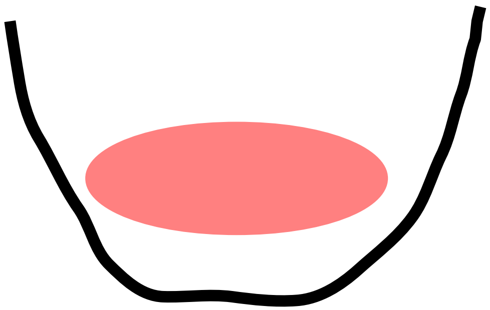
Change of potentials

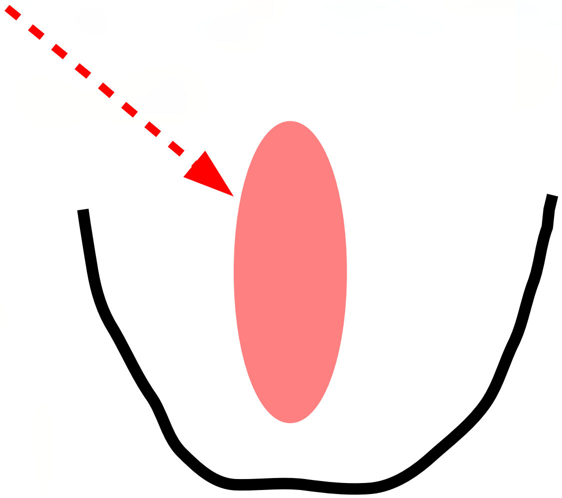
Excitation ?

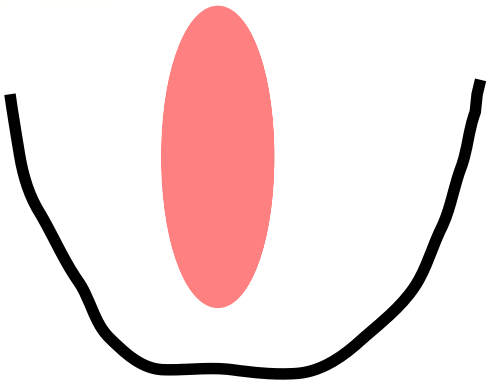
→ Induced potentials

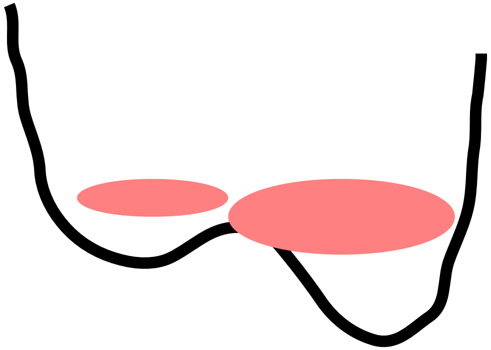


Change of potentials



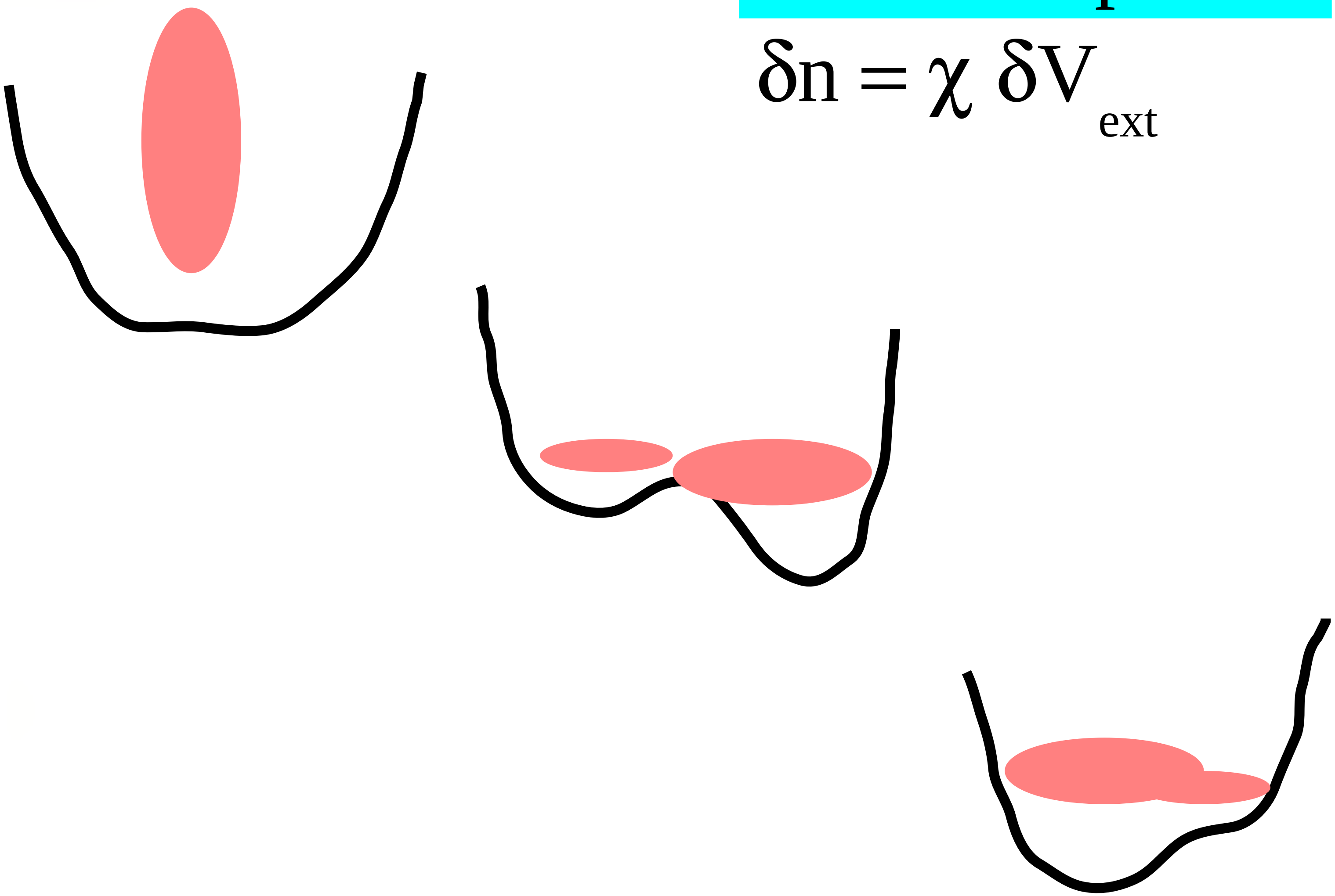






Linear response:

$$\delta n = \chi\, \delta V_{ext}$$



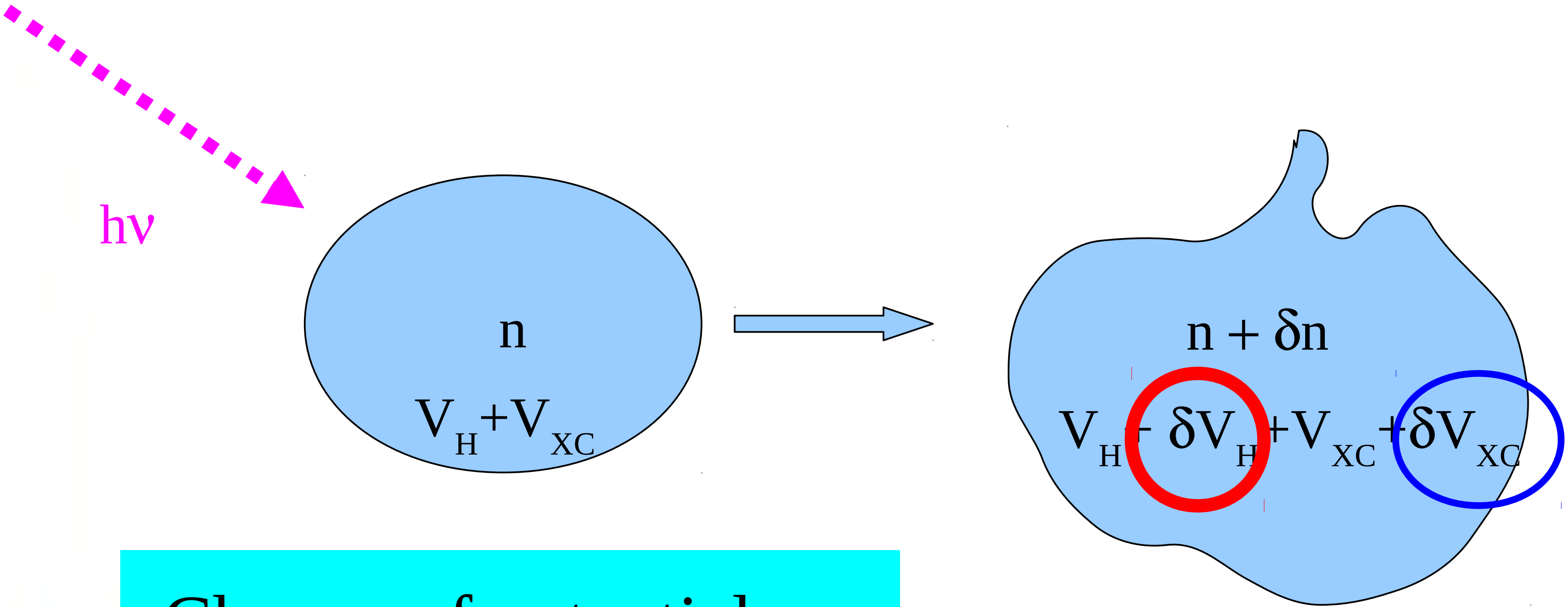
$$\chi = \chi_0 + \chi_0\, [\delta V/\delta n]\, \chi_0 + \chi_0\, [\delta V/\delta n]\, \chi_0\, [\delta V/\delta n]\, \chi_0 + \chi_0\, [\delta V/\delta n] \ldots\ldots\ldots\ldots$$

$$\chi = \chi_0 + \chi_0\, [\delta V/\delta n]\, \chi$$

Dyson equation

Excitation ?

→ Induced potentials



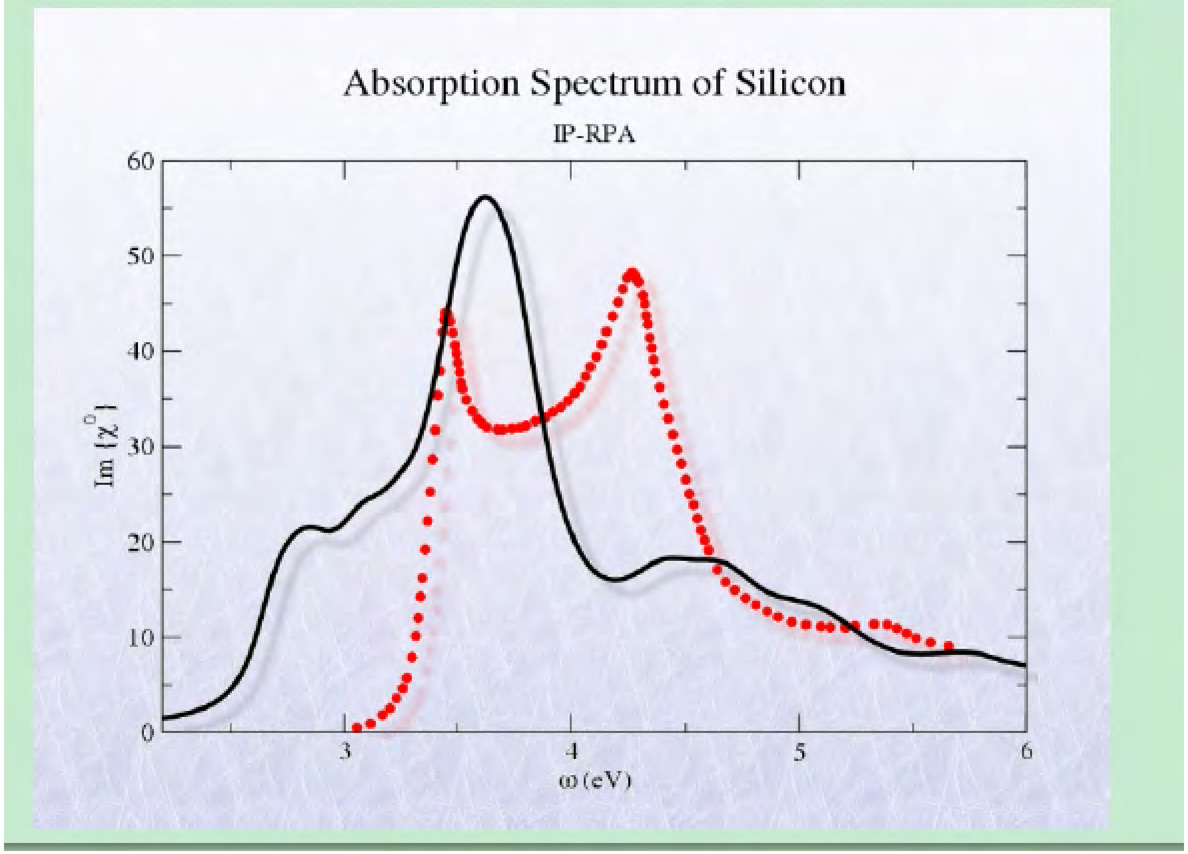
Change of potentials

RPA

TDLDA, ...

Approximation

All this for nothing???



By F. Sottile

Strategy

→ Define an effective quantity from which we can get exp. values
(in principle, and reasonably well also in practice)

→ Build an auxiliary system that yields this quantity

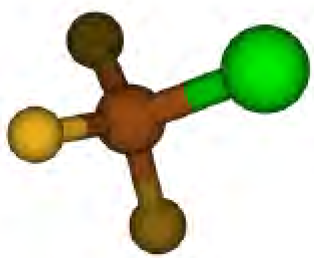
→ Use it to calulate observables

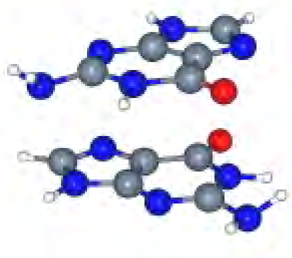
→ For response functions (variations of observables),
also take into account variations of the potentials

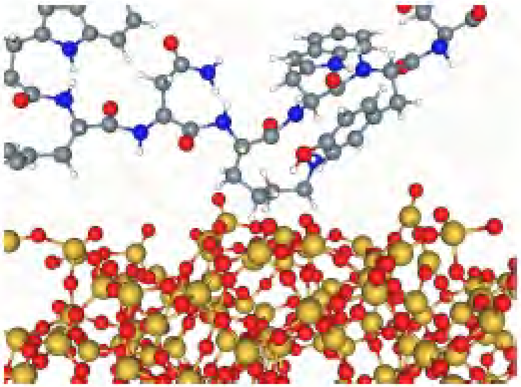
→ More flexible effective quantity: G

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

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



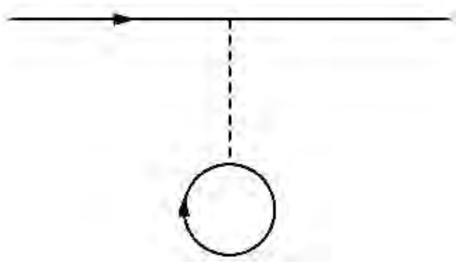


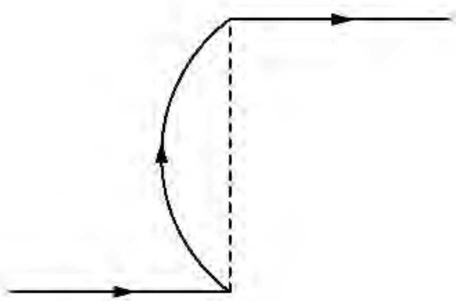


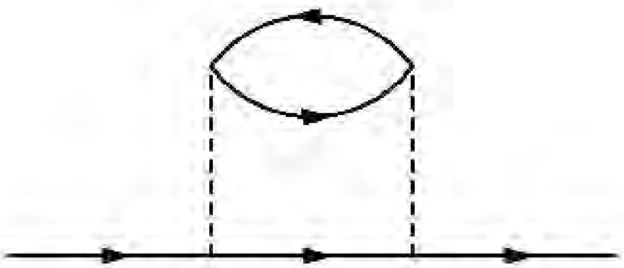
→ Propagators. *G yields all exp. values of 1-body operators*

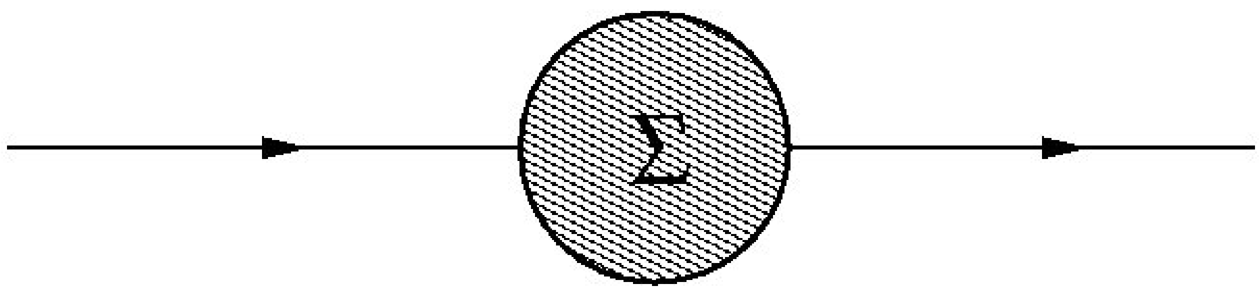
$$\mathcal{G}(1,2) = -i \langle T[\psi(1)\psi^{\dagger}(2)] \rangle \qquad 1=(r_1,\sigma_1,t_1)$$

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









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

Same procedure for a Green's function:

$$[\omega - H]\, G^{tot} = I, \tag{4}$$

$$H = \begin{bmatrix} H_S & H_{SR} \\ H_{RS} & H_R \end{bmatrix}, \quad G^{tot} = \begin{bmatrix} G_S & G_{SR} \\ G_{RS} & G_R \end{bmatrix}, \quad \text{and} \quad I = \begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix}, \tag{5}$$

$$G_S(\omega) = \left(\omega - H_S - H_{SR}\, [\omega - H_R]^{-1}\, H_{RS}\right)^{-1}$$

or

$$G_S(\omega) = \left([G_S^0(\omega)]^{-1} - H_{SR}\; G_R^0(\omega)\; H_{RS}\right)^{-1}$$

Equation for a small part of a Green's function:

$$G_S(\omega) = \left([G_S^0(\omega)]^{-1} - \Sigma_S(\omega)\right)^{-1}, \tag{6}$$

with

$$\Sigma_S(\omega) = [G_S^0(\omega)]^{-1} - [G_S(\omega)]^{-1} = H_{SR}\, G_R^0(\omega)\, H_{RS}. \tag{7}$$

Σ_S is the self-energy: it contains the effect of "the rest"!

$$G(\mathbf{x}, \mathbf{x}', \omega) = \left\langle N, 0 \middle| \psi(\mathbf{x}) \left(\omega - \hat{H} + E_N + i\eta\right)^{-1} \psi^\dagger(\mathbf{x}') \middle| N, 0 \right\rangle + \cdots .$$

The rest are other excitations!

→ The effective world:

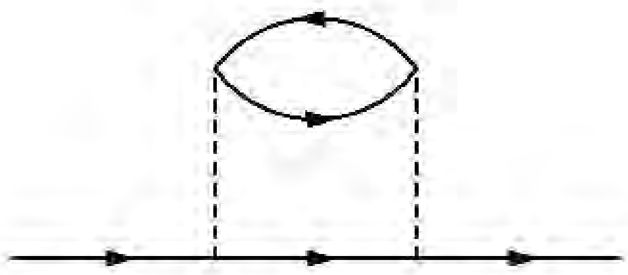
$$\left(-\frac{1}{2}\boldsymbol{\nabla}^2 + v_{\text{eff}}(\mathbf{r})\right)\psi_i(\mathbf{r}) = \varepsilon_i\psi_i(\mathbf{r})$$

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

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

Direct access to electron addition and removal spectra (bandstructure, lifetimes, satellites,....,density,...total Energy..)

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

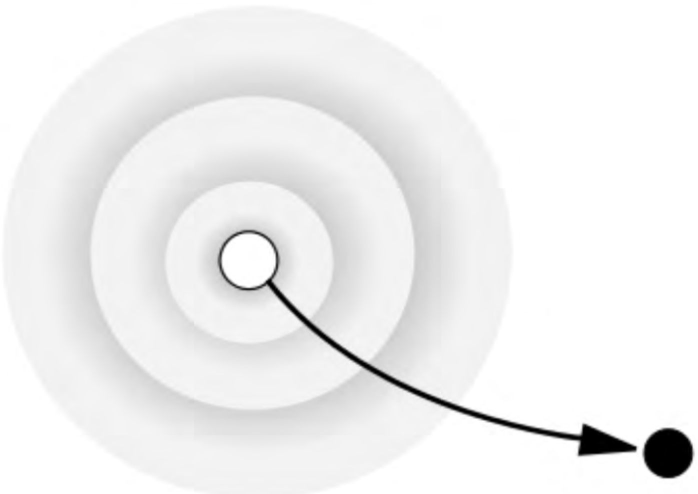


+ ....

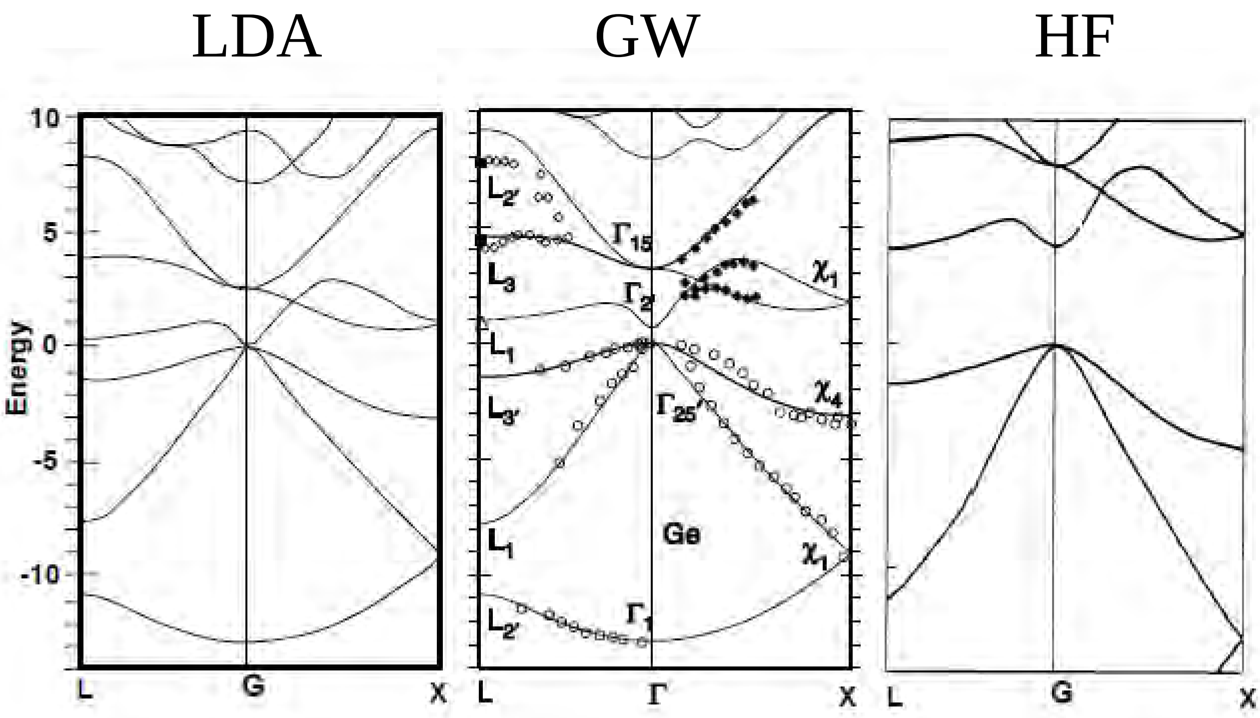
$\rightarrow \Sigma \sim i\,\mathcal{W}\mathcal{G}$ "GW"

L. Hedin (1965)

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



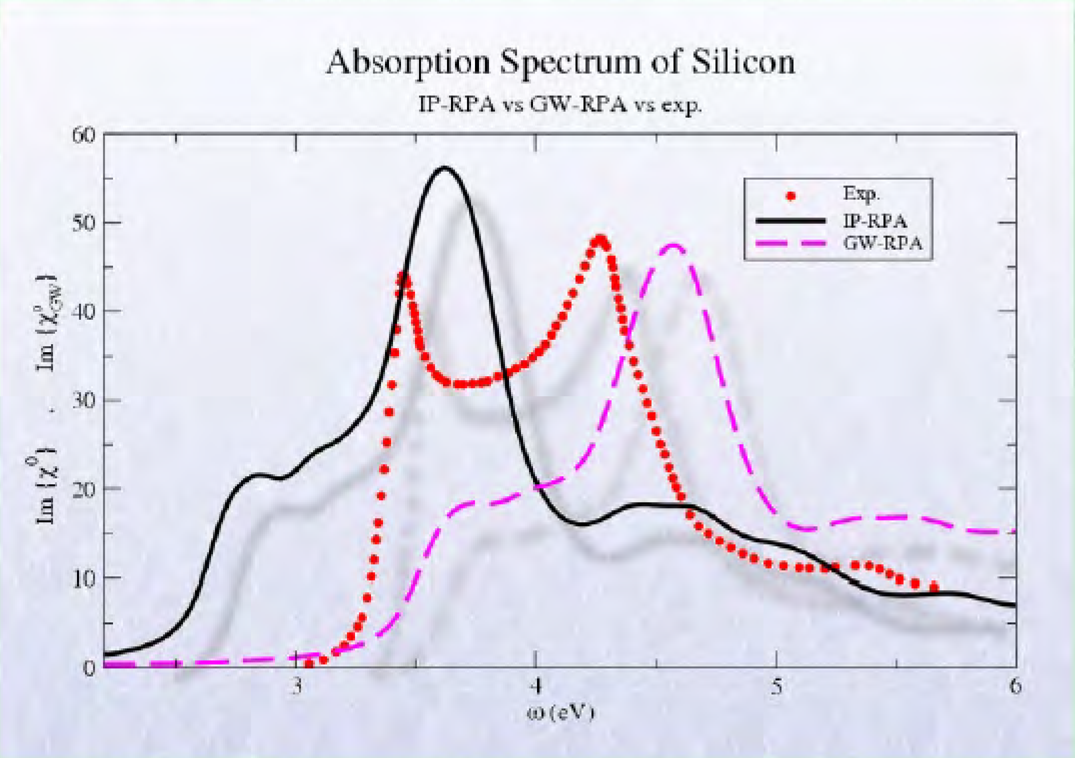
GW today: standard for bandstructures



Bandstructure of germanium, theory versus experiment

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

Spectra in GW-RPA



Strategy

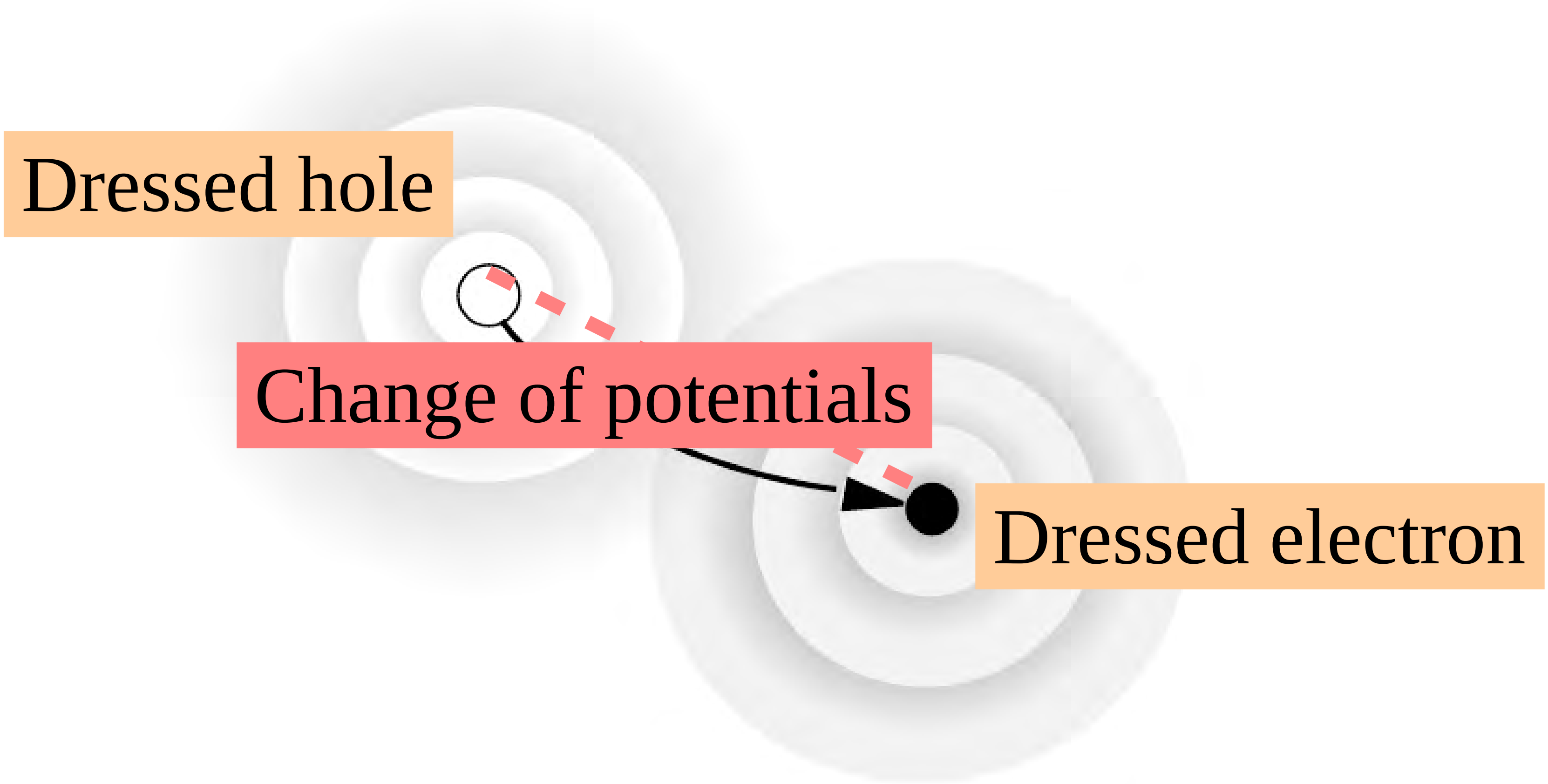
→ Define an effective quantity from which we can get exp. values *(in principle, and reasonably well also in practice)*

→ Build an auxiliary system that yields this quantity

→ Use it to calulate observables

→ For response functions (variations of observables),
also take into account variations of the potentials

→ What is missing?



TD-GFT

Time evolution of the MBPT equations?

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

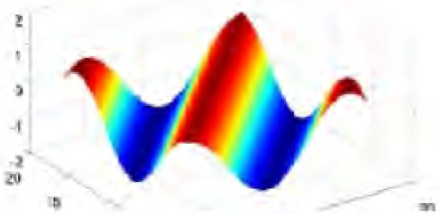
$G(t,t')$ $\Sigma(t,t')$

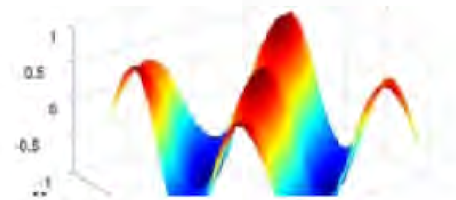
Tough!!!!!!!

TD-.... ?

Time evolution of the MBPT equations?

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



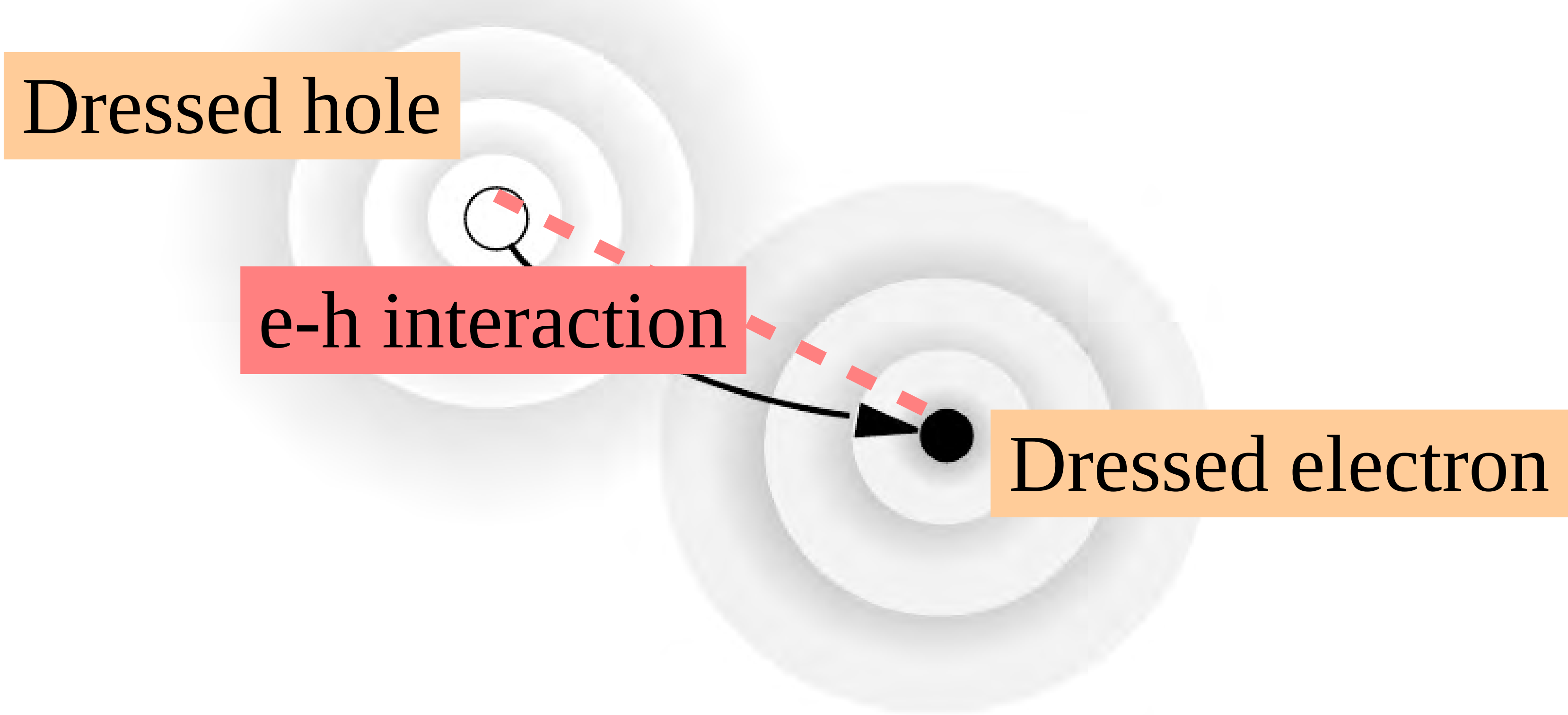


A. Stan, N. E. Dahlen, and R. van Leeuwen, J. Chem. Phys. 130, 2009.

N. E. Dahlen, R. van Leeuwen, and A. Stan,
in Progress in Nonequilibrium Green's Functions III, Vol. 35 of J. Phys. Conference Series, edited by M Bonitz and A Filinov, 2006, pp. 340–348, conference on Progress in Nonequilibrium Greens Functions III, Kiel, Germany, AUG, 2005.

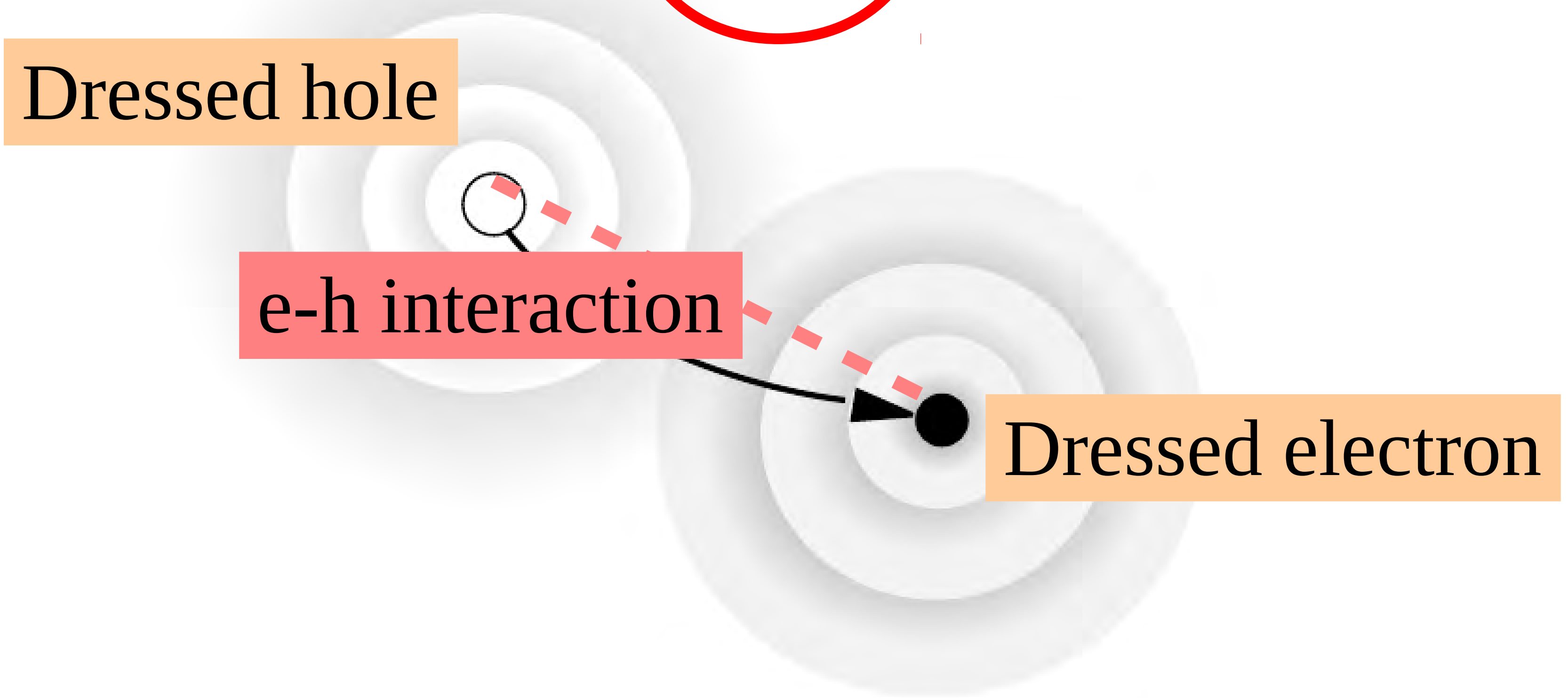
→ Linear response: Bethe-Salpeter equation

$$\chi = \chi_0 + \chi_0 \, [\delta V/\delta n] \, \chi$$



→ Linear response: Bethe-Salpeter equation

$$\chi = \chi_0 + \chi_0 \, [\delta\Sigma/\delta G] \, \chi$$



$$\delta n(r,t) = \chi(rt;r't')\delta V_{ext}(r't')$$

$$\chi(rt;r't') = \chi_0(rt;r't') + \chi_0(rt;r_1t_1)[\delta V(r_1t_1)/\delta n(r_2t_2)]\,\chi\,(r_2t_2;r't')$$

$$r_1t_1 \rightarrow 1$$

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

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

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

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

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

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

Comparison with Linear Response quantities

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

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

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

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

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

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

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

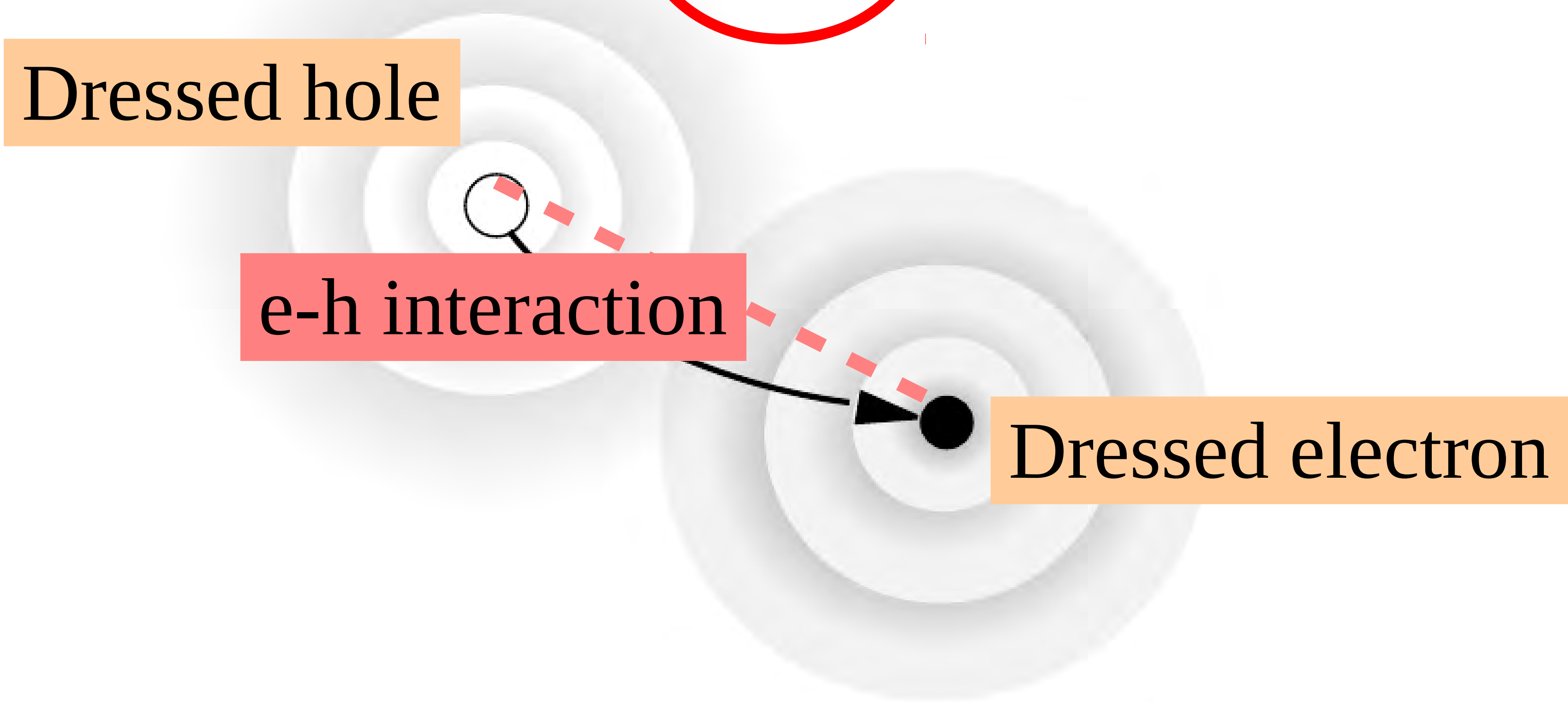
Hartree-Fock: $\Sigma(5,6) = iv(5,6)G(5,6^+)$

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

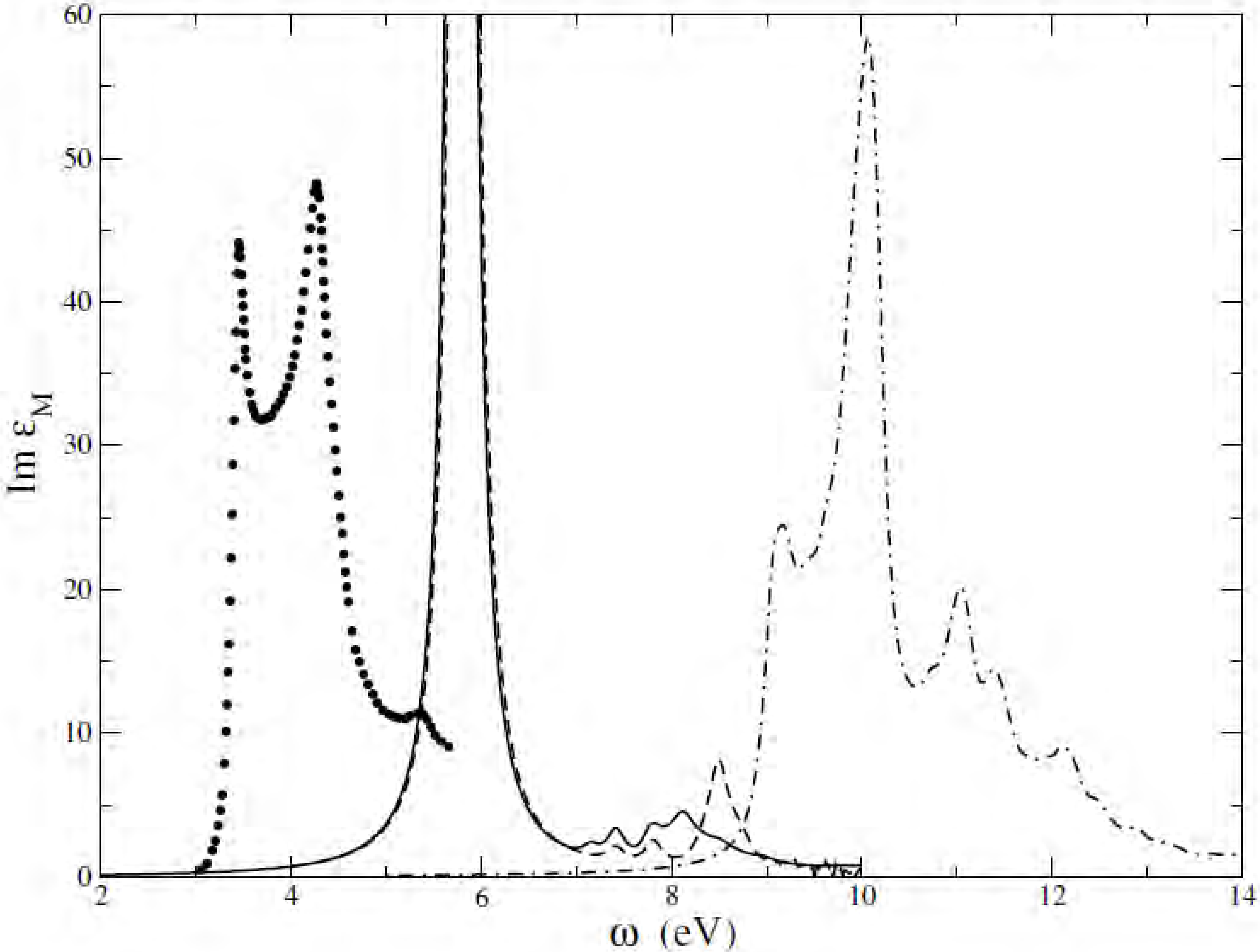
$n(r,r';t) = -iG(rt,r't^+)$

→ Linear response: Bethe-Salpeter equation

$$\chi = \chi_0 + \chi_0\, [\delta\Sigma/\delta G]\, \chi$$



Silicon



F. Bruneval et al.

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

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

$\Rightarrow$ **Standard Bethe-Salpeter equation (Time-Dependent Screened Hartree-Fock)**

$$L = GG + GG\,[v - W]\,L$$

$\Rightarrow$ 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

Mixing of transitions

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

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

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

(or inverting)

BSE - creating and diagonalizing a (big) matrix

$$\Rightarrow \quad H^{exc}_{(vc)(v'c')} A_\lambda^{(v'c')} = E_\lambda^{exc} A_\lambda^{(vc)}$$

$$\Rightarrow \quad L_{(vc)}^{(v'c')}(\omega) = \sum_\lambda \frac{A_\lambda^{(vc)} A_\lambda^{*(v'c')}}{\omega - E_\lambda^{exc} + i\eta}$$

Spectrum in BSE (only resonant)

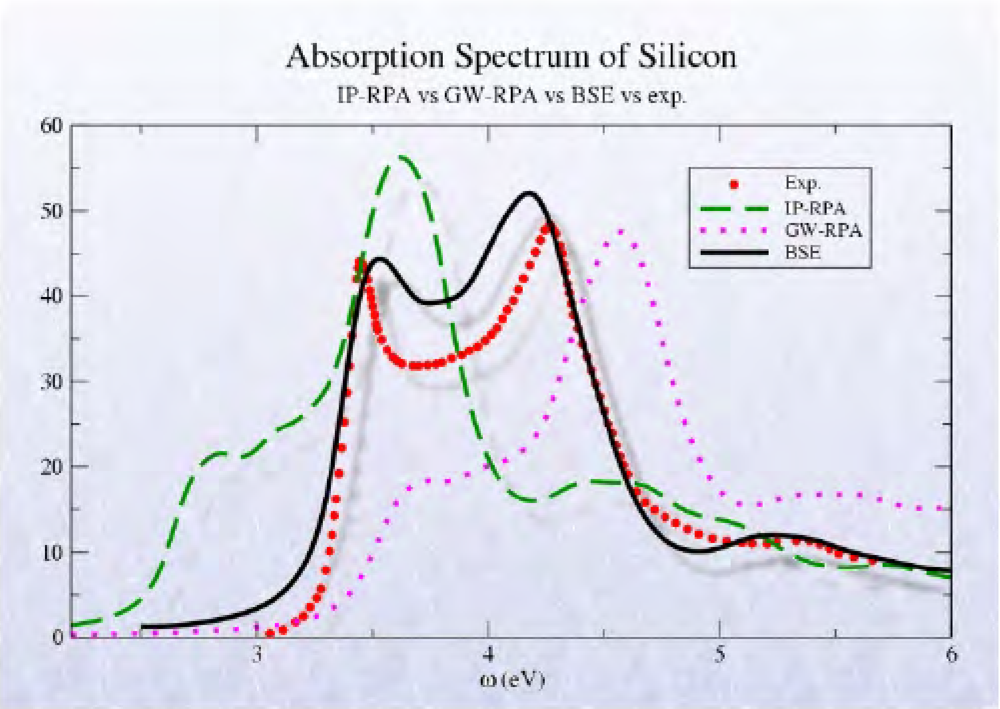
$$\mathrm{Abs}^{\mathrm{BSE}}(\omega) = Im\,\langle L(\omega)\rangle = \sum_{\lambda}\left|\sum_{vc} A_{\lambda}^{(vc)}\langle c|D|v\rangle\right|^{2}\delta\left(\omega - E_{\lambda}^{exc}\right)$$

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

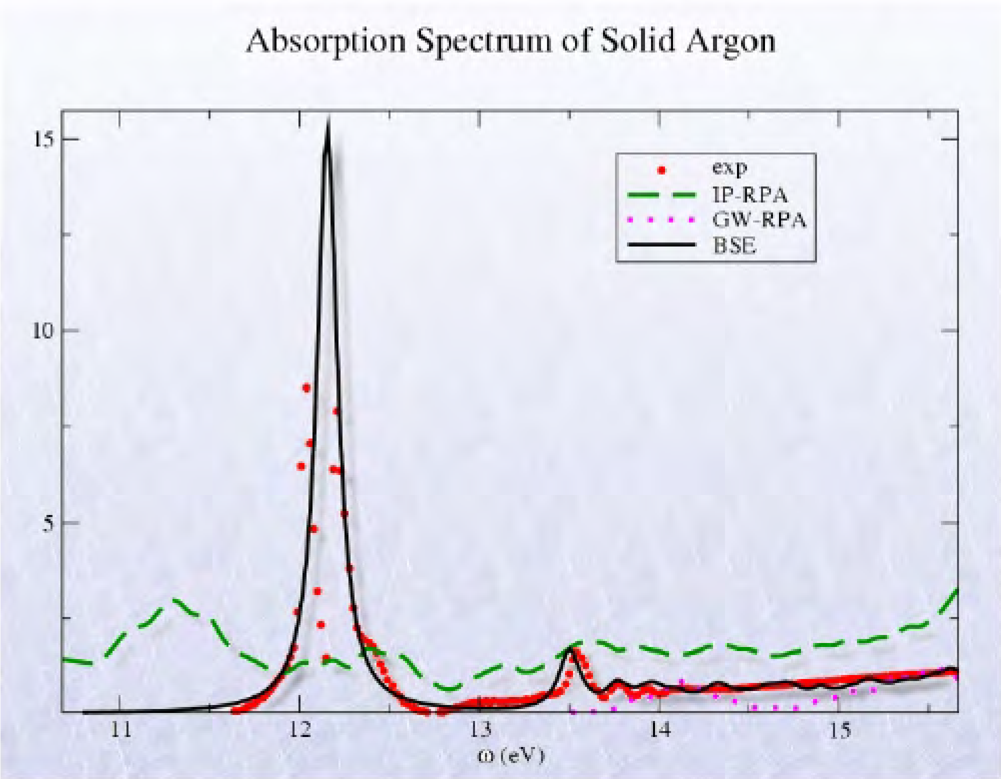
BSE in practice

Standard Approximations for BSE

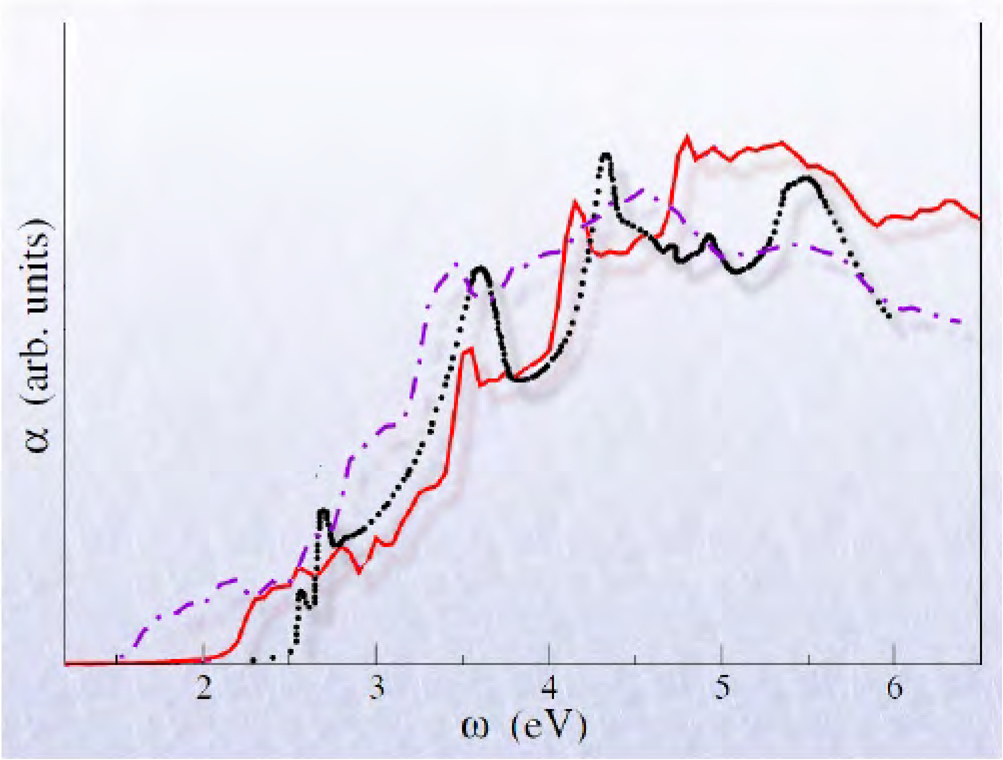
- Ground-state
  - pseudopotential
  - V_{xc} local density approximation
- Quasi-particle Many-Body Theory
  - GW approximation for Σ
  - W rpa, plasmon-pole model
  - $\psi_{\mathrm{GW}} = \phi_{\mathrm{KS}}$
- Bethe-Salpeter equation
  - $\dfrac{\delta W}{\delta G} = 0$
  - W rpa, static
  - only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



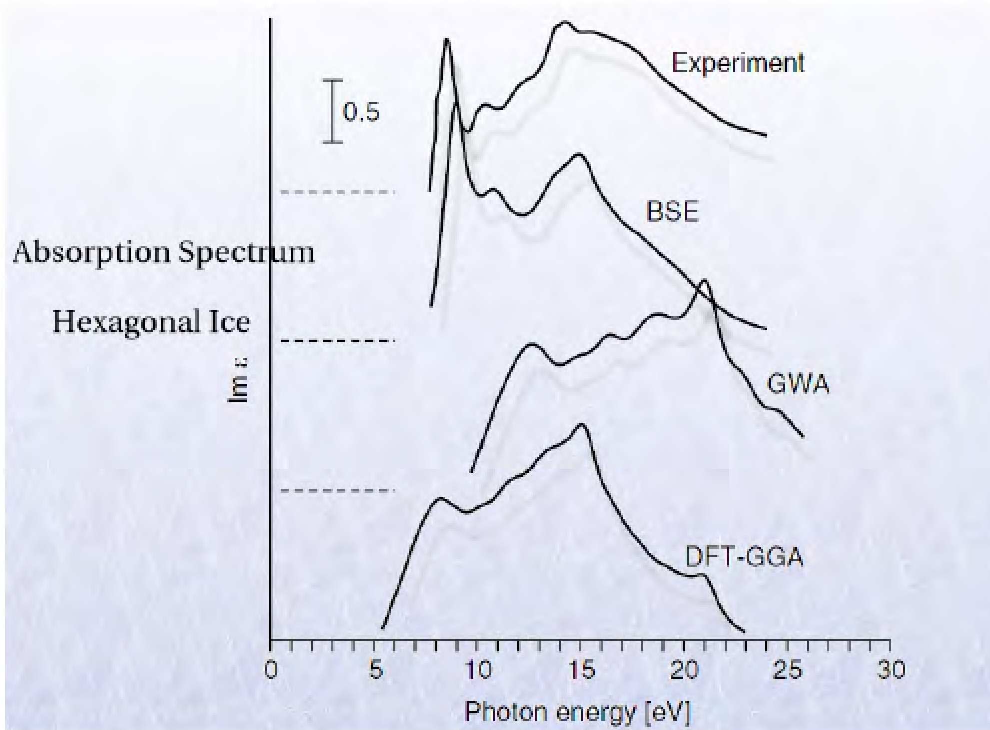
Albrecht *et al.*, PRL **80**, 4510 (1998)



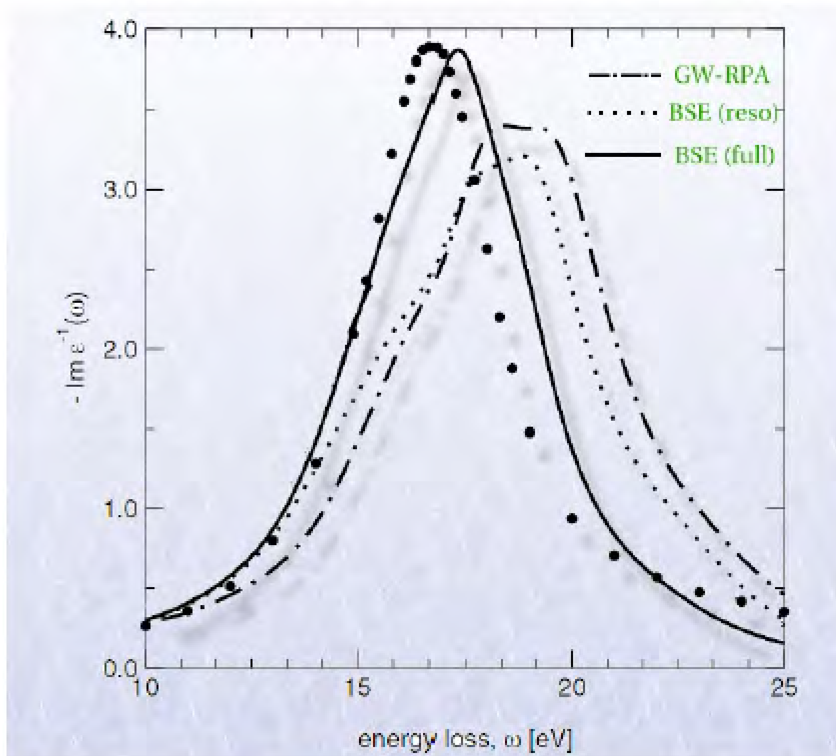
Sottile, Marsili, *et al.*, PRB (2007).



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

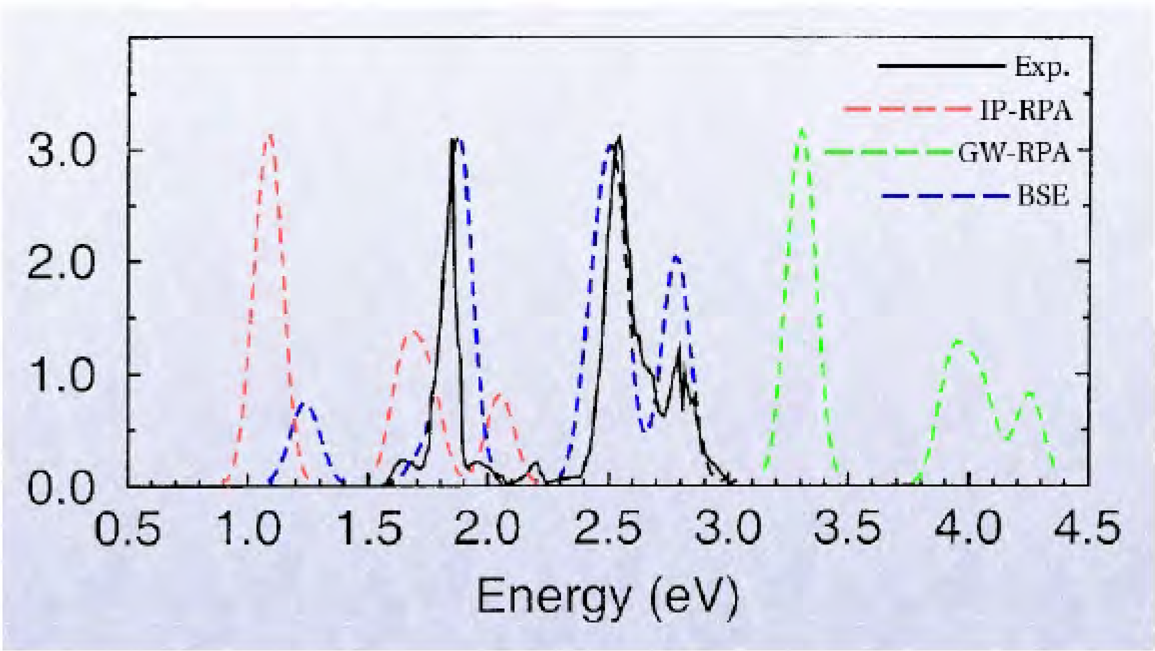


Hahn *et al.*, PRL **94**, 37404 (2005)

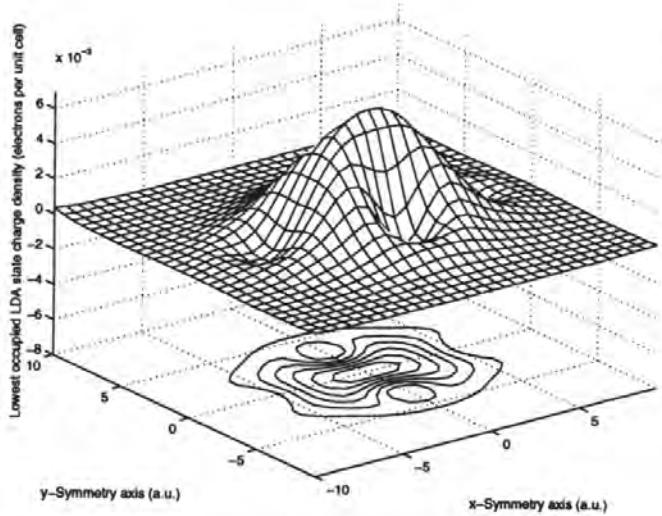


Olevano and Reining, PRL **86**, 5962 (2001)

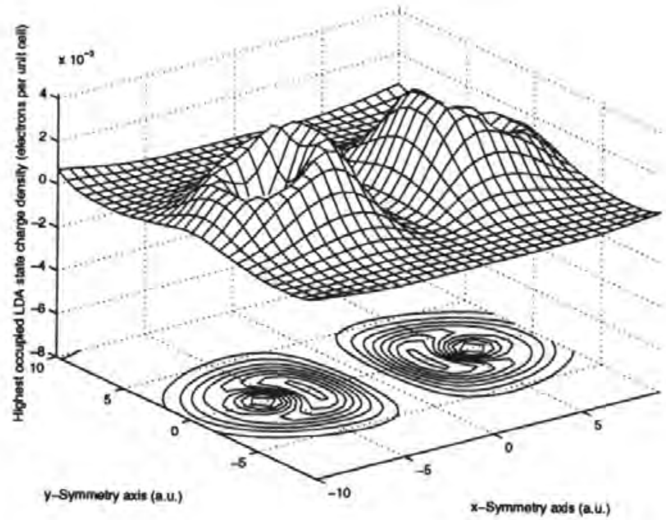
Bethe-Salpeter equation results: Molecule (Na_4)



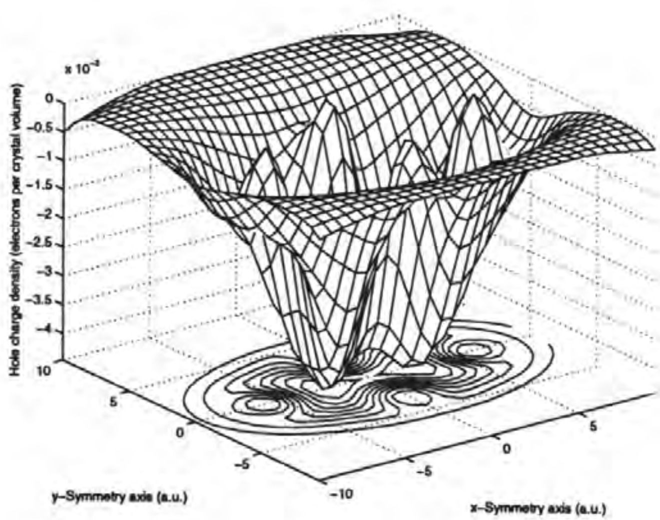
Onida *et al.*, PRL **75**, 818 (1995)



(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.

Notes:

* Finite systems and correlation

* The “bandgap problem”

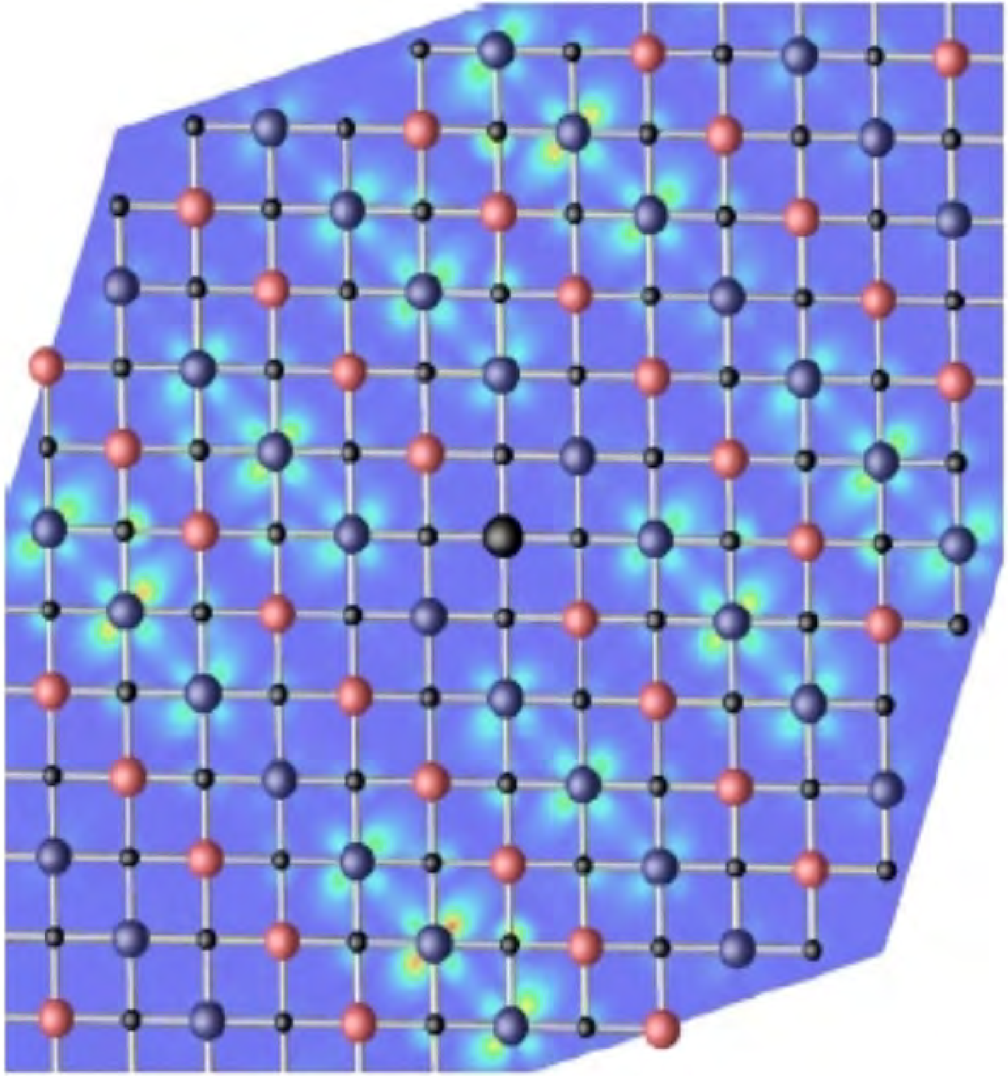
* BSE yields a two-particle correlation function

*$\Sigma = iGW\Gamma$

Notes:

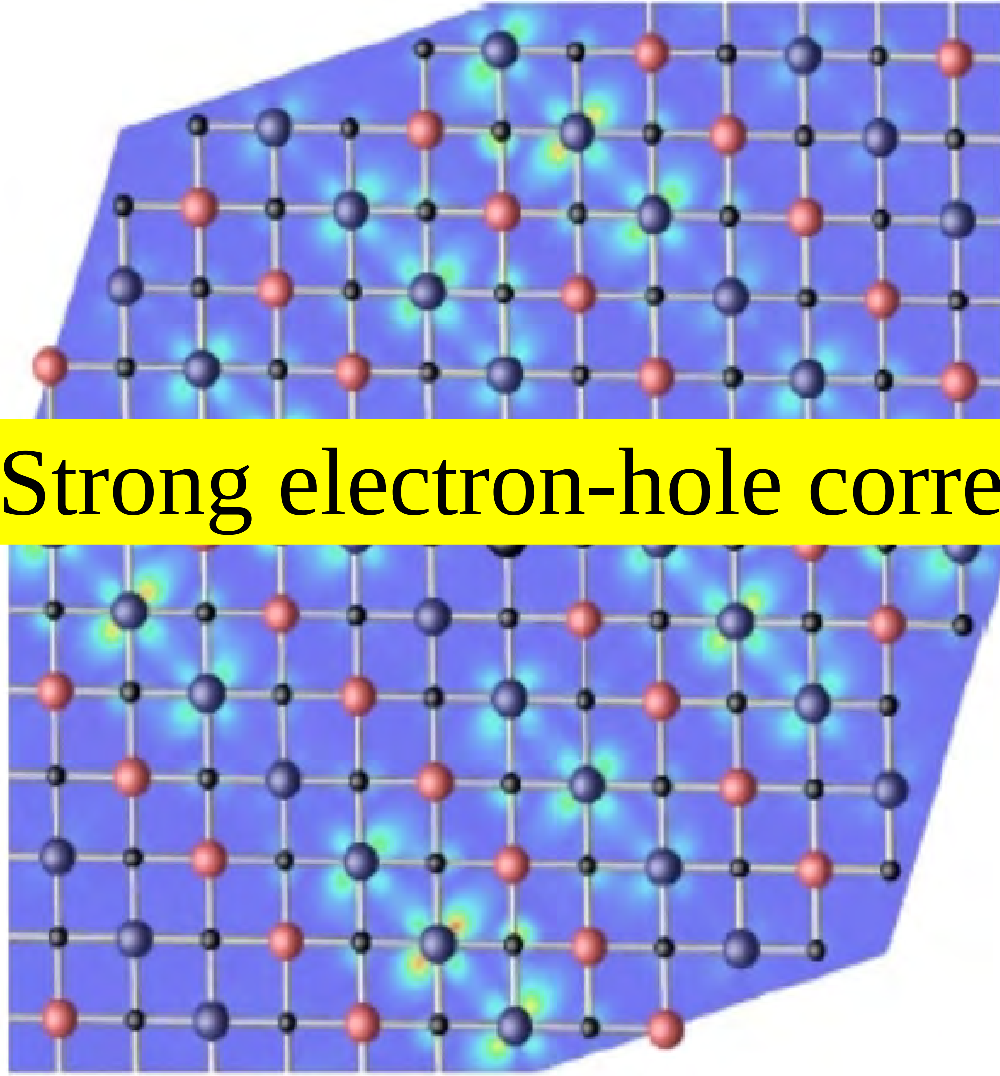
* Finite systems versus correlation in extended systems

MnO



C. Rödl, F. Fuchs, J. Furthmüller, and F. Bechstedt, Phys. Rev. B **77**, 184408 (2008)

MnO



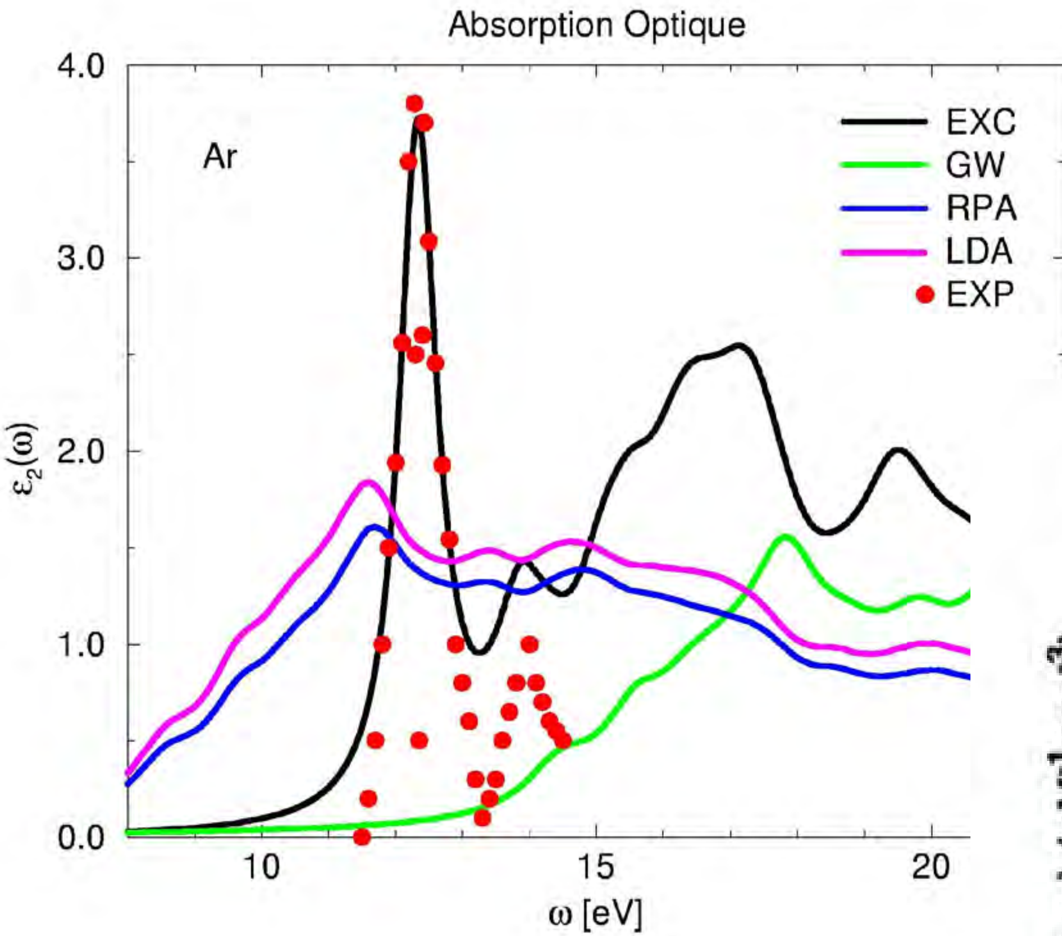
Strong electron-hole correlation!

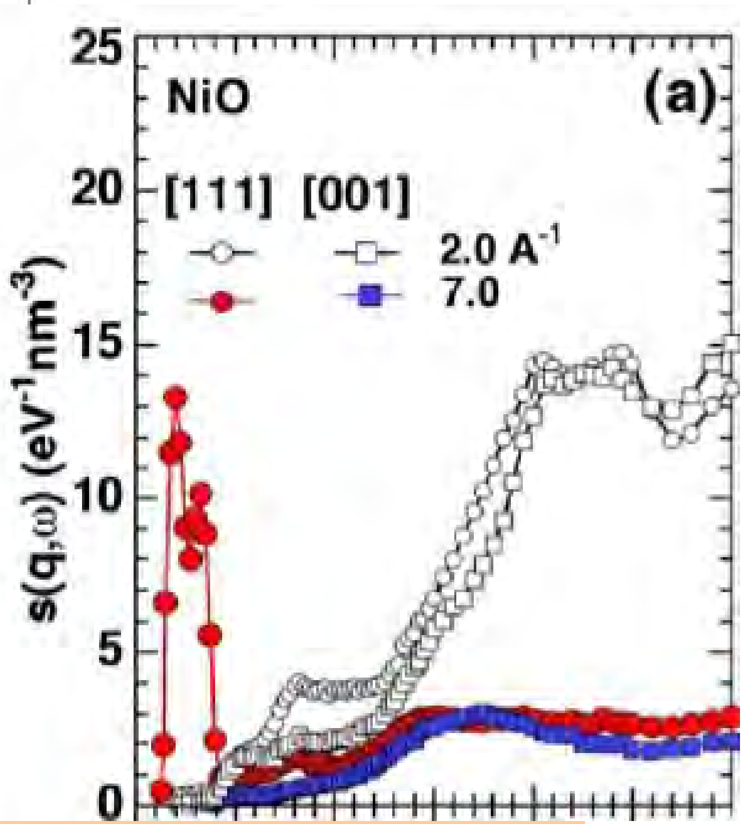
C. Rödl, F. Fuchs, J. Furthmüller, and F. Bechstedt, Phys. Rev. B **77**, 184408 (2008)

Notes:

* Finite systems and correlation

* The “bandgap problem”



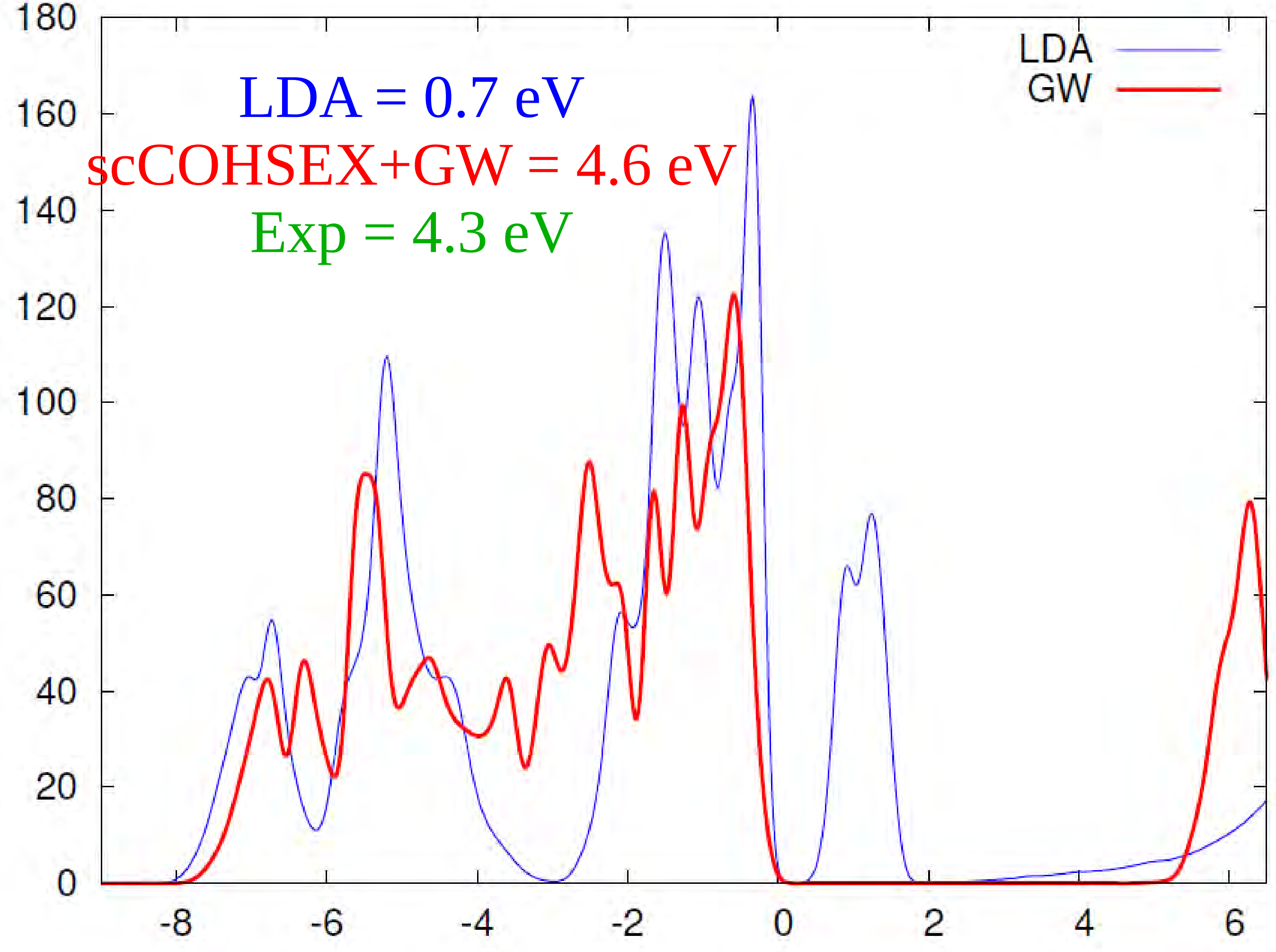


V. Olevano et al. (2000)
(bulk silicon 1998)

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

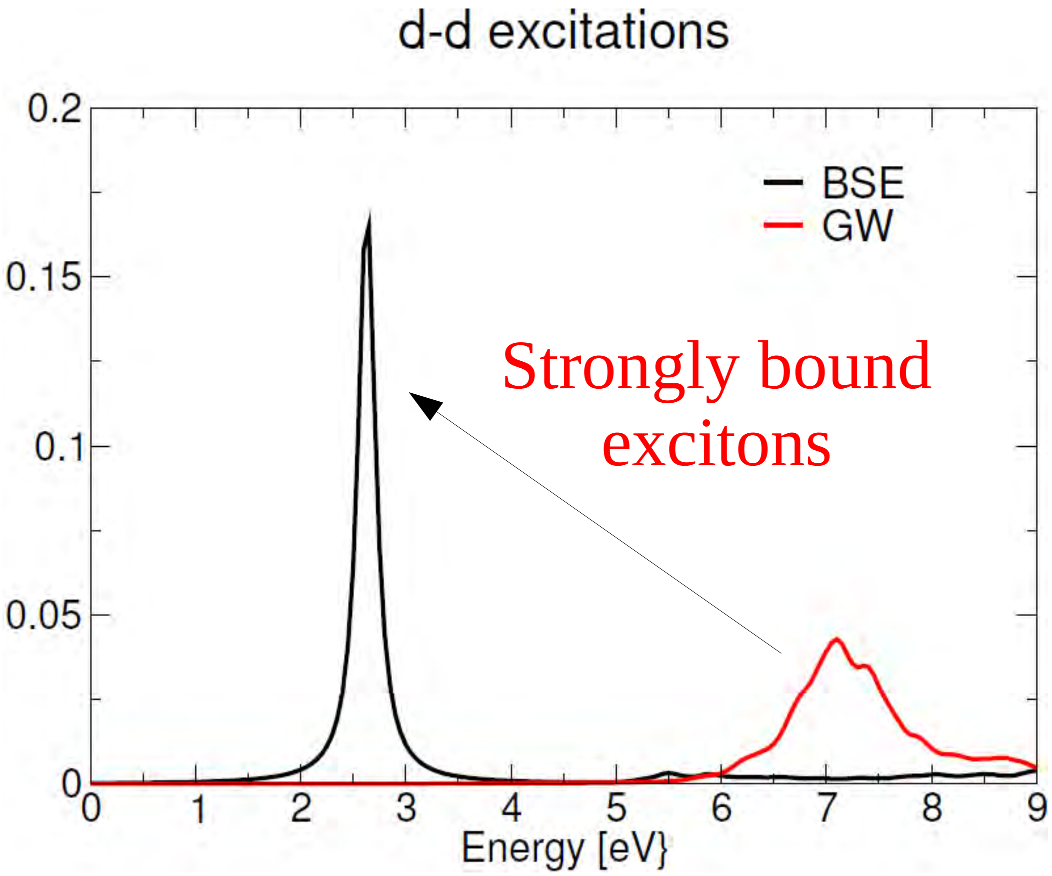
Exciton: Lee, Hsueh, Ku, PRB 82, 081106 (2010)

NiO: density of states



M. Guzzo, Master thesis (2008)

NiO: dd excitations

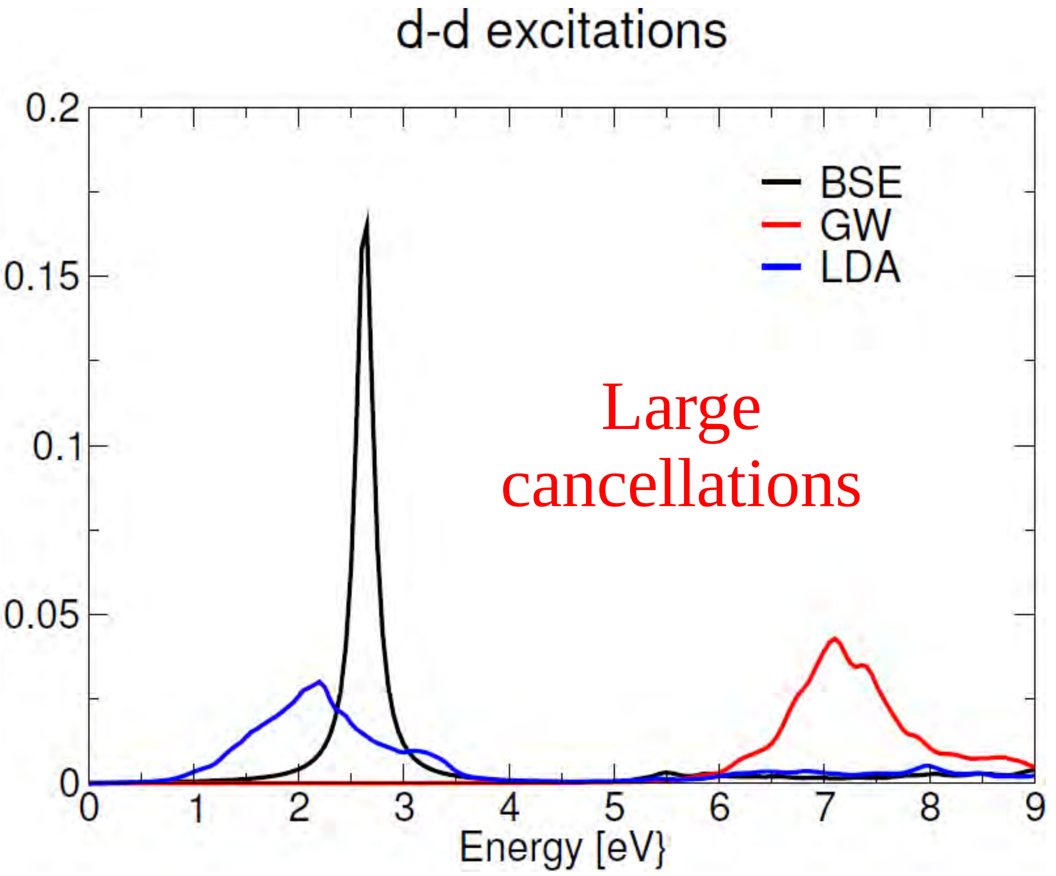


Q ~ 8 Å^{-1} [111]

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”

* BSE yields a two-particle correlation function

Comparison with Linear Response quantities

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

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

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

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

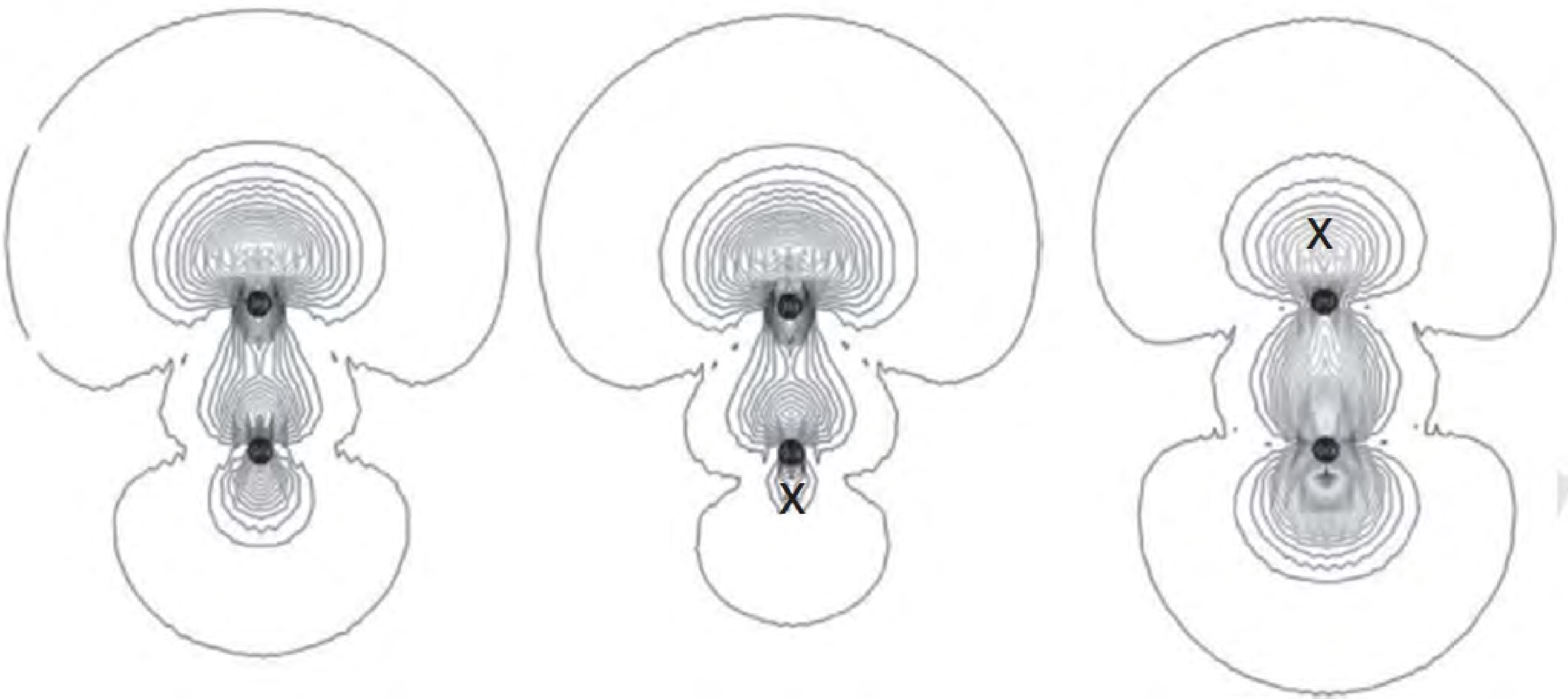
Other combinations yield other correlations

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

Bethe-Salpeter Equation

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

CO molecule



Noguchi, Ishii, Ohno, J. Chem. Phys. 125, 114108 (2006)

Notes:

* Finite systems and correlation

* The “bandgap problem”

* BSE yields a two-particle correlation function

* $\Sigma = iGW\Gamma$

The electron-hole problem : LR

Hedin's equations

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

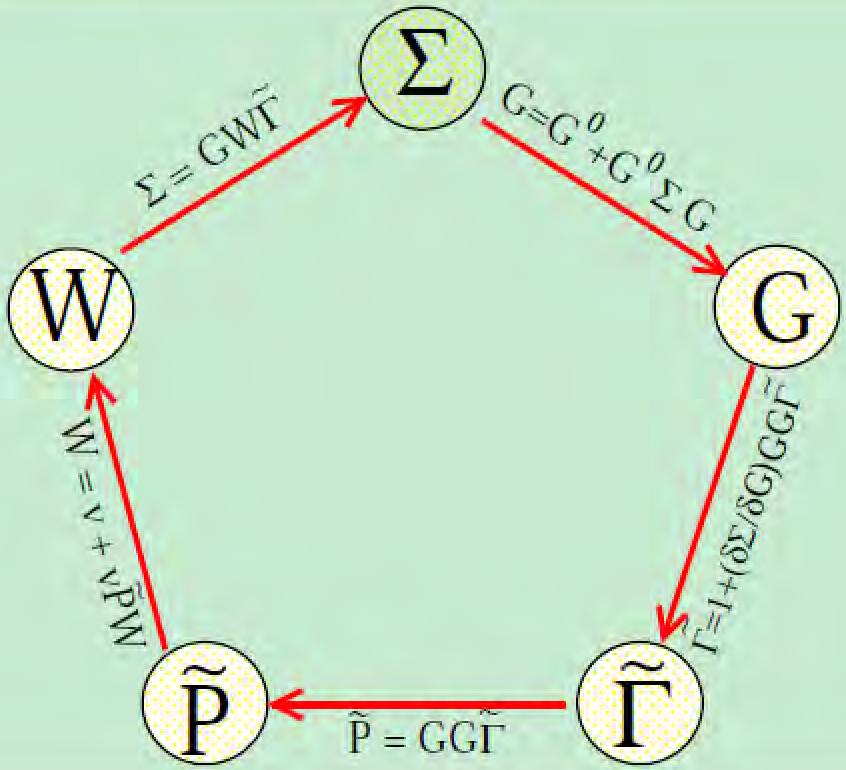
$$G(1,2) = G^0(1,2) + \int d(34) G^0(1,3) \Sigma(3,4) G(4,2)$$

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

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

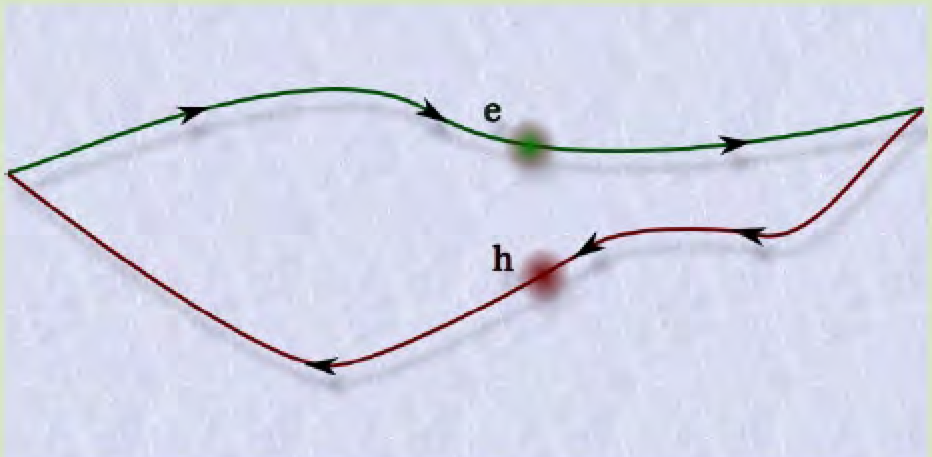
$$W(1,2) = v(1,2) + \int d(34) v(1,3) \tilde{P}(3,4) W(4,2)$$

Hedin's pentagon



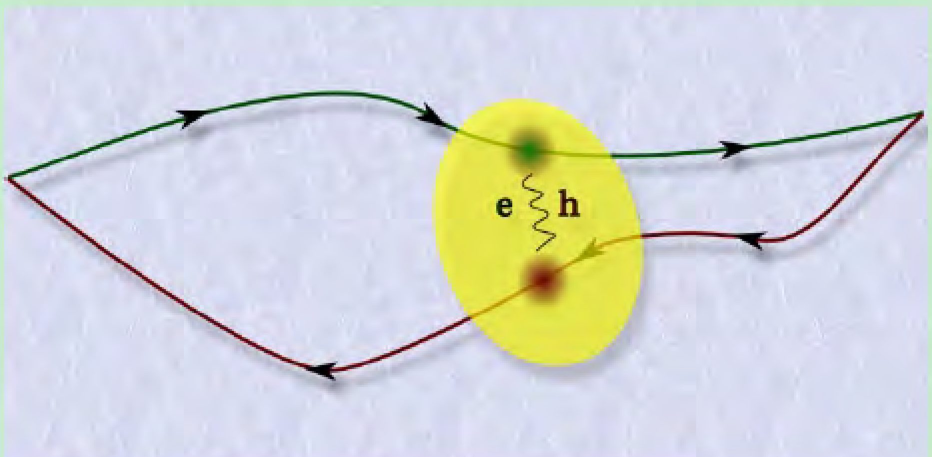
GG Polarizability

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



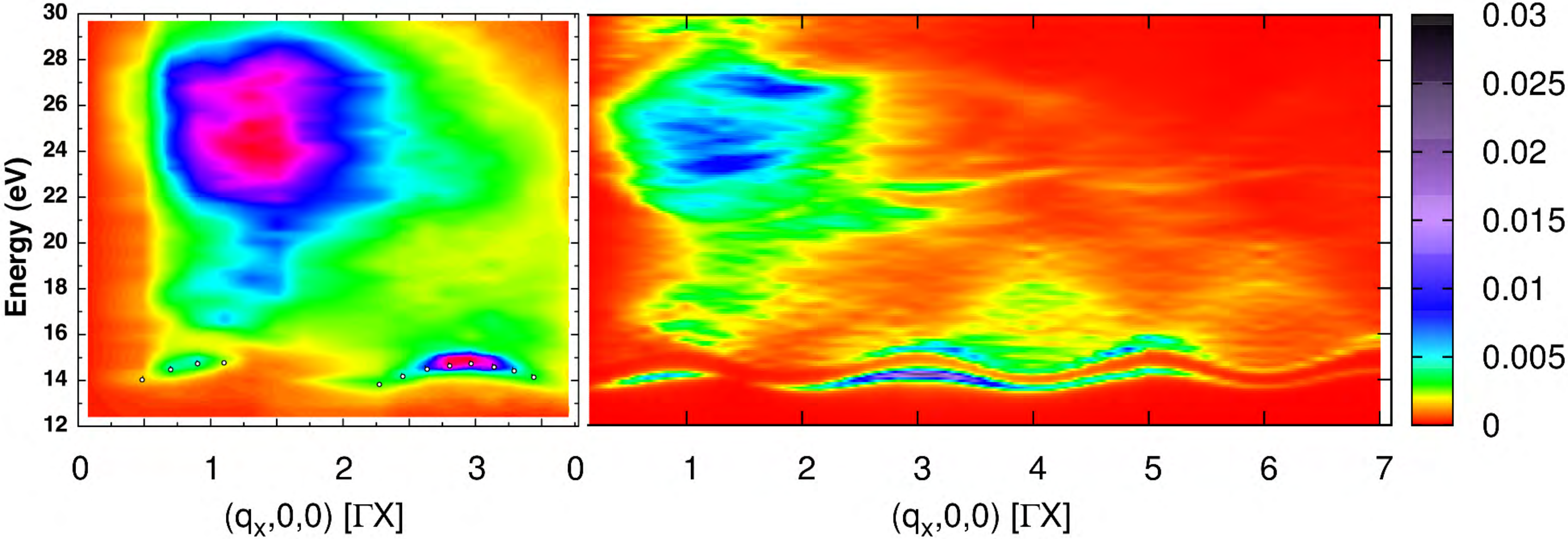
GGΓ Polarizability

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



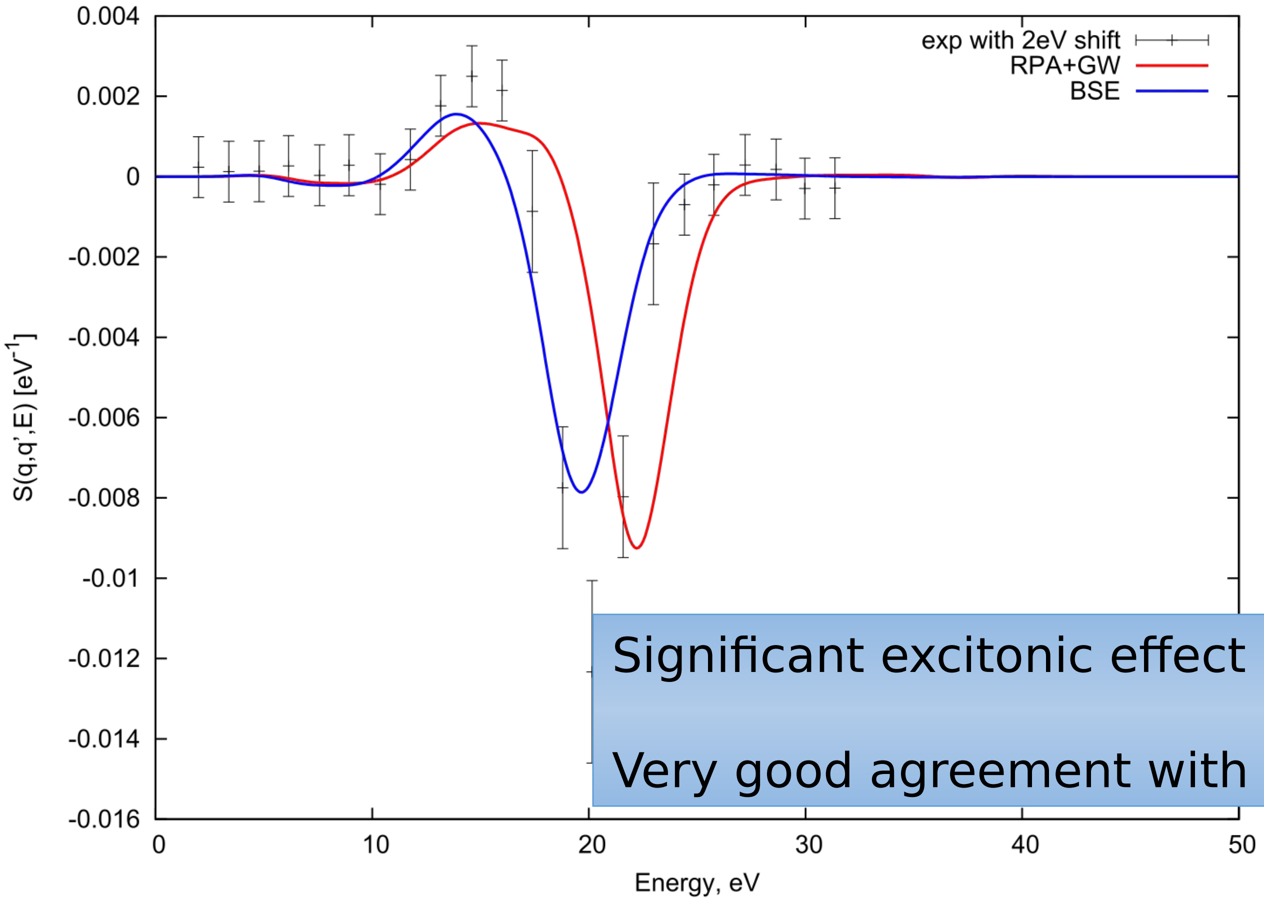
$$\tilde{\Gamma}(1,2,3) = \delta(1,2)\delta(1,3) + \\ + \int d(4567)\frac{\delta\Sigma(1,2)}{\delta G(4,5)} G(4,6)G(7,5)\tilde{\Gamma}(6,7,3)$$

Exciton dispersion in LiF



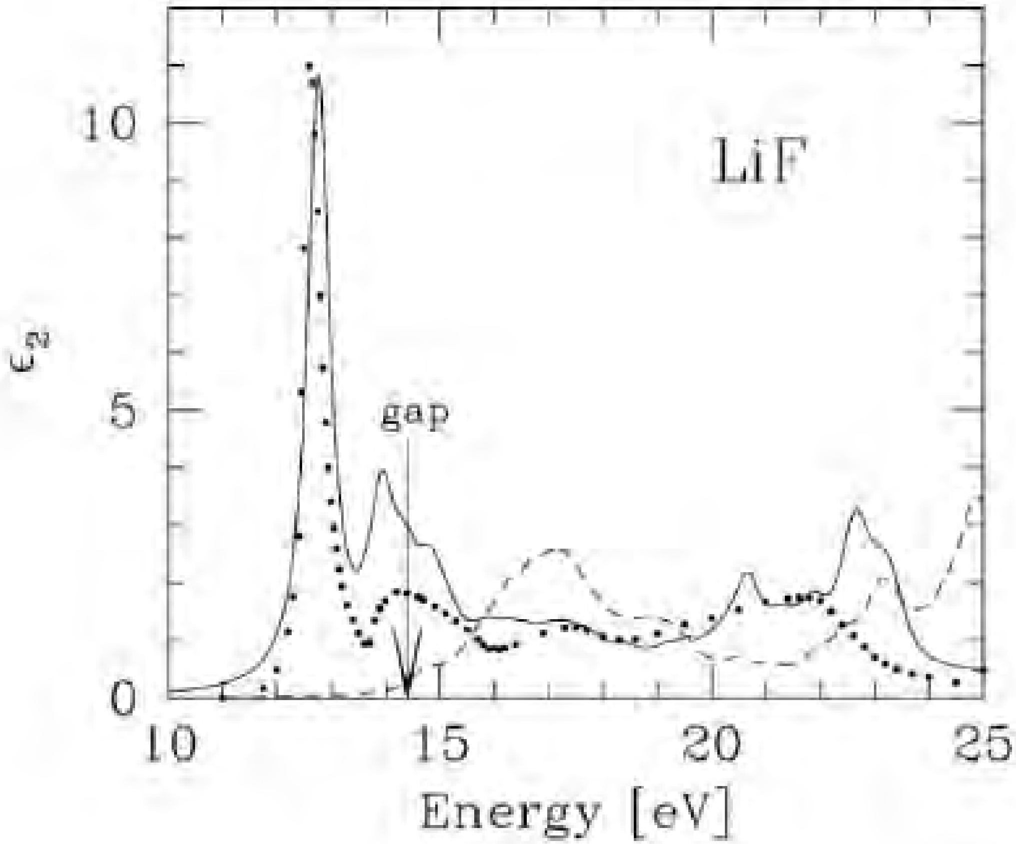
M. Gatti and F. Sottile, Phys. Rev. B 88, 155113
Exp. P. Abbamonte et al., Proc. Natl. Acad. Sci. USA 105, 12159 (2008).

PhD thesis Igor Reshetnyak (23.9.2015)



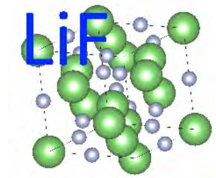
Significant excitonic effect

Very good agreement with experiment

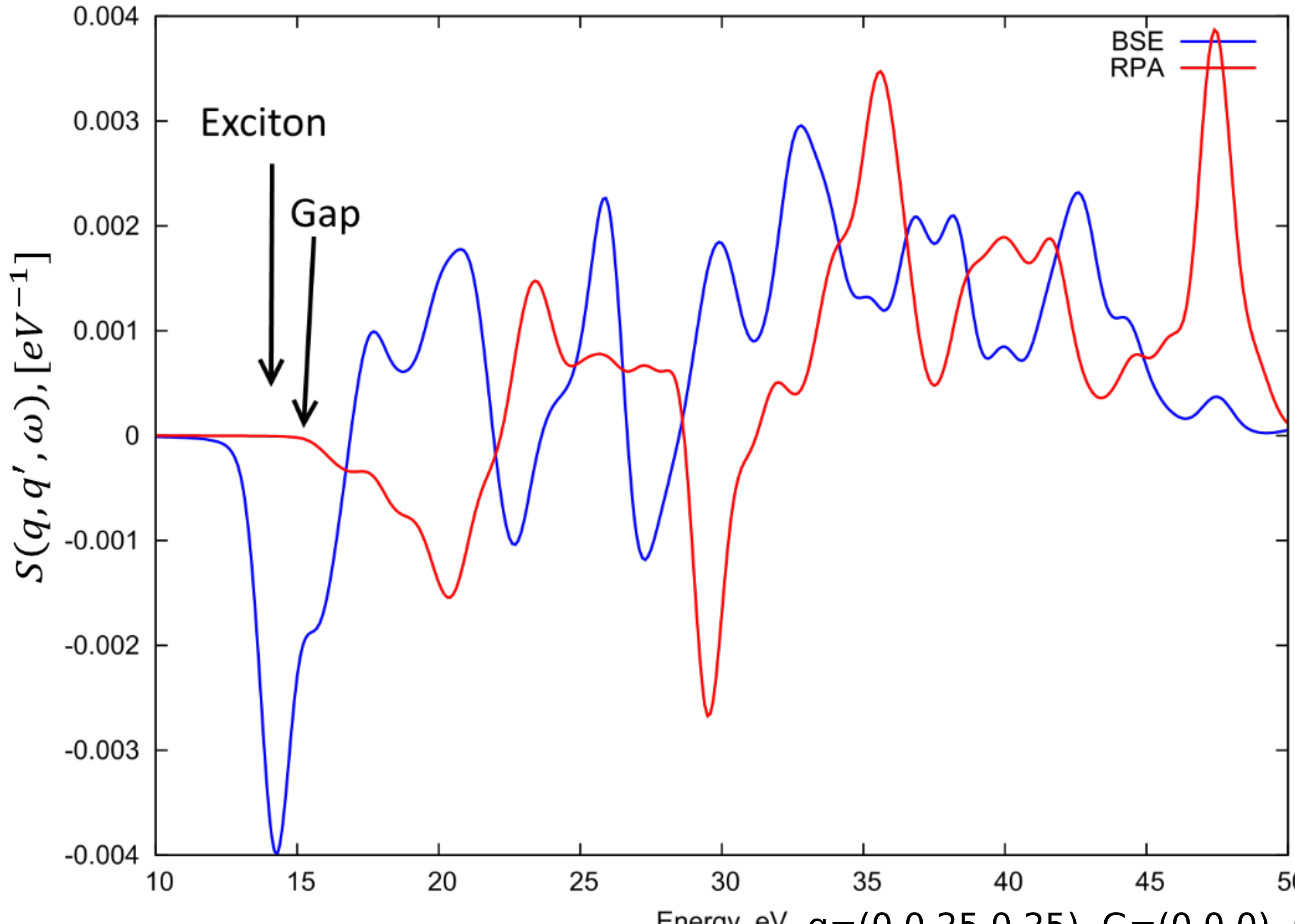


Rohlfing and Louie, PRL 81, 2312 (1998)

Mixed Dynamic Structure Factor



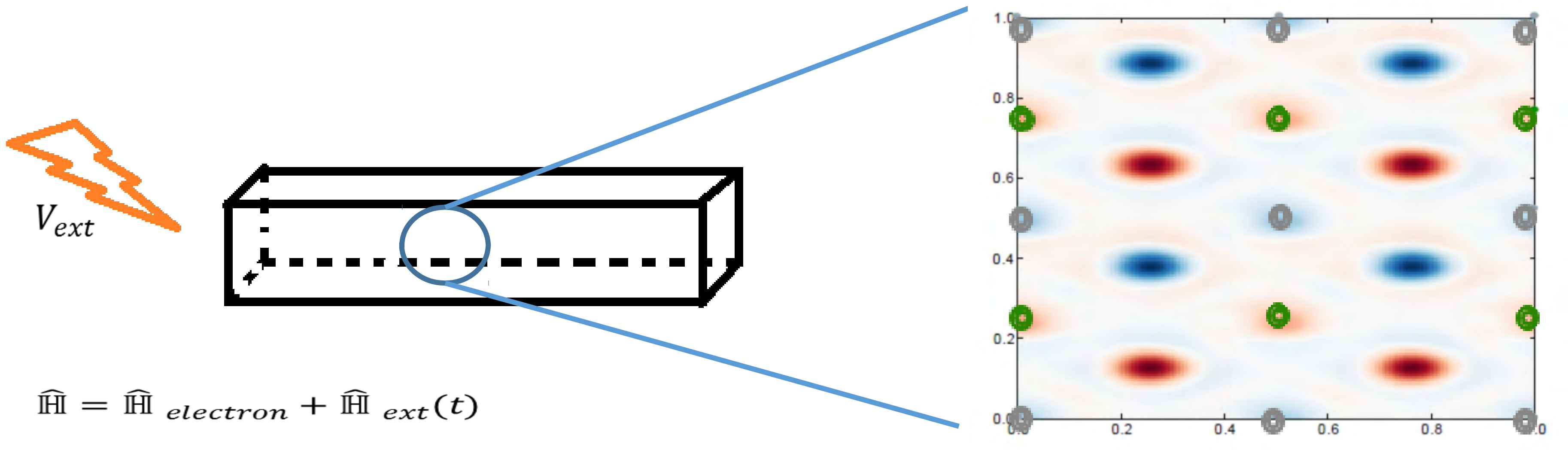
Strongly bound exciton visible



q=(0,0.25,0.25), G=(0,0,0), G’=(1,1,1)

PhD thesis Igor Reshetnyak (23.9.2015)

What can we do with it?
For example, induced charges



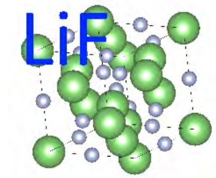
$$\hat{\mathbb{H}} = \hat{\mathbb{H}}_{electron} + \hat{\mathbb{H}}_{ext}(t)$$

(exchange)

In linear response:

$$\delta n(\mathbf{r},t) = \int dt' d\mathbf{r}' \chi(\mathbf{r},\mathbf{r}',t-t') v_{ext}(\mathbf{r}',t')$$

Ralf Hambach
Giulia Pegolotti
Claudia Roedl
Igor Reshetnyak

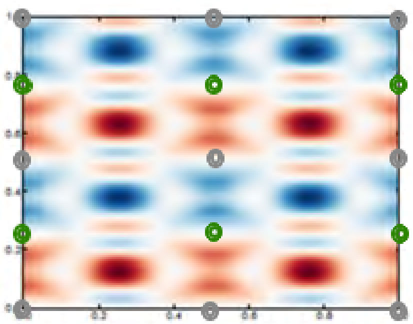


Induced Charges

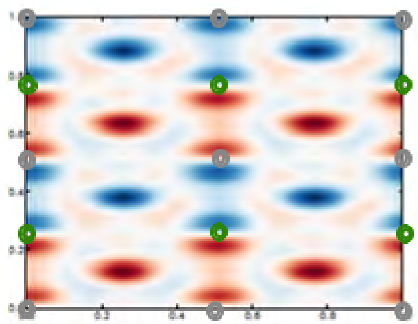
$$\delta n(\boldsymbol{r},t) = \int d\omega \sum_{\boldsymbol{q},\boldsymbol{G},\boldsymbol{G}'} \chi_{\boldsymbol{G},\boldsymbol{G}'}(\boldsymbol{q},\omega) V_{ext}(\boldsymbol{q}+\boldsymbol{G}',\omega) e^{i(\boldsymbol{q}+\boldsymbol{G})\boldsymbol{r}} e^{-i\omega t}$$

Plane-wave external potential

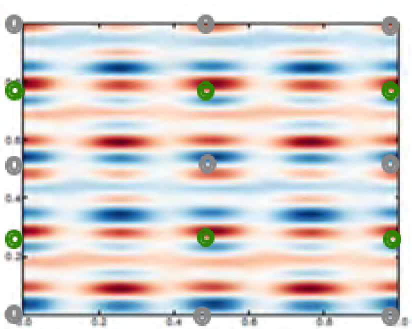
Excitonic effects visible



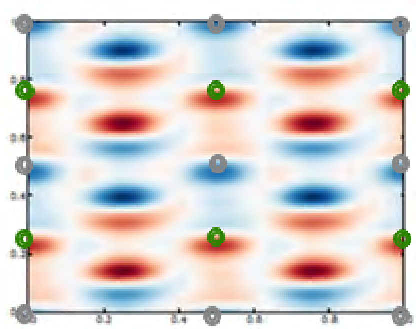
RPA susceptibility, $\omega = 14eV$



RPA susceptibility, $\omega = 25.6eV$



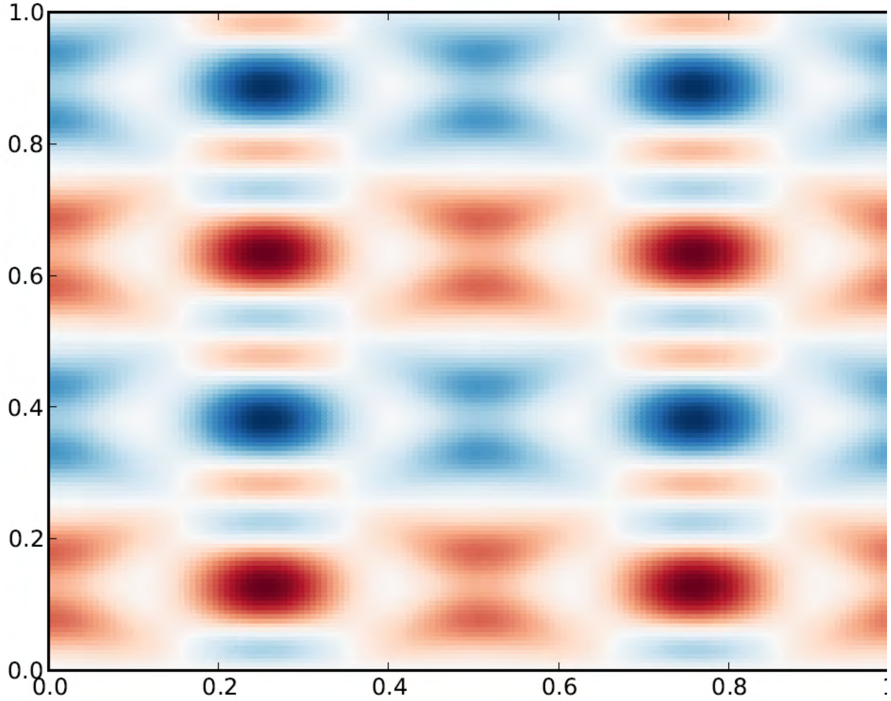
BSE susceptibility, $\omega = 14eV$



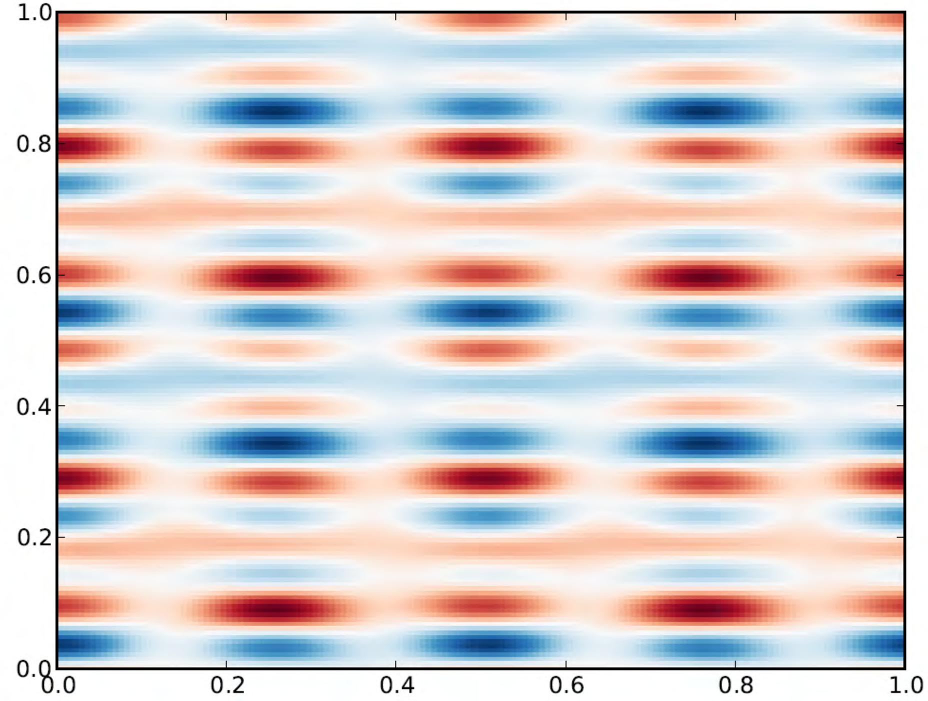
BSE susceptibility, $\omega = 25.6eV$

PhD thesis I. Reshetnyak

[1] P. Abbamonte et al. *Phys. Rev. Lett.* 2004. [2] P. Abbamonte et al. *Advanced Materials* 2010.



RPA



BSE

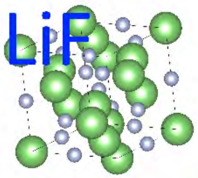
At 14.1 eV

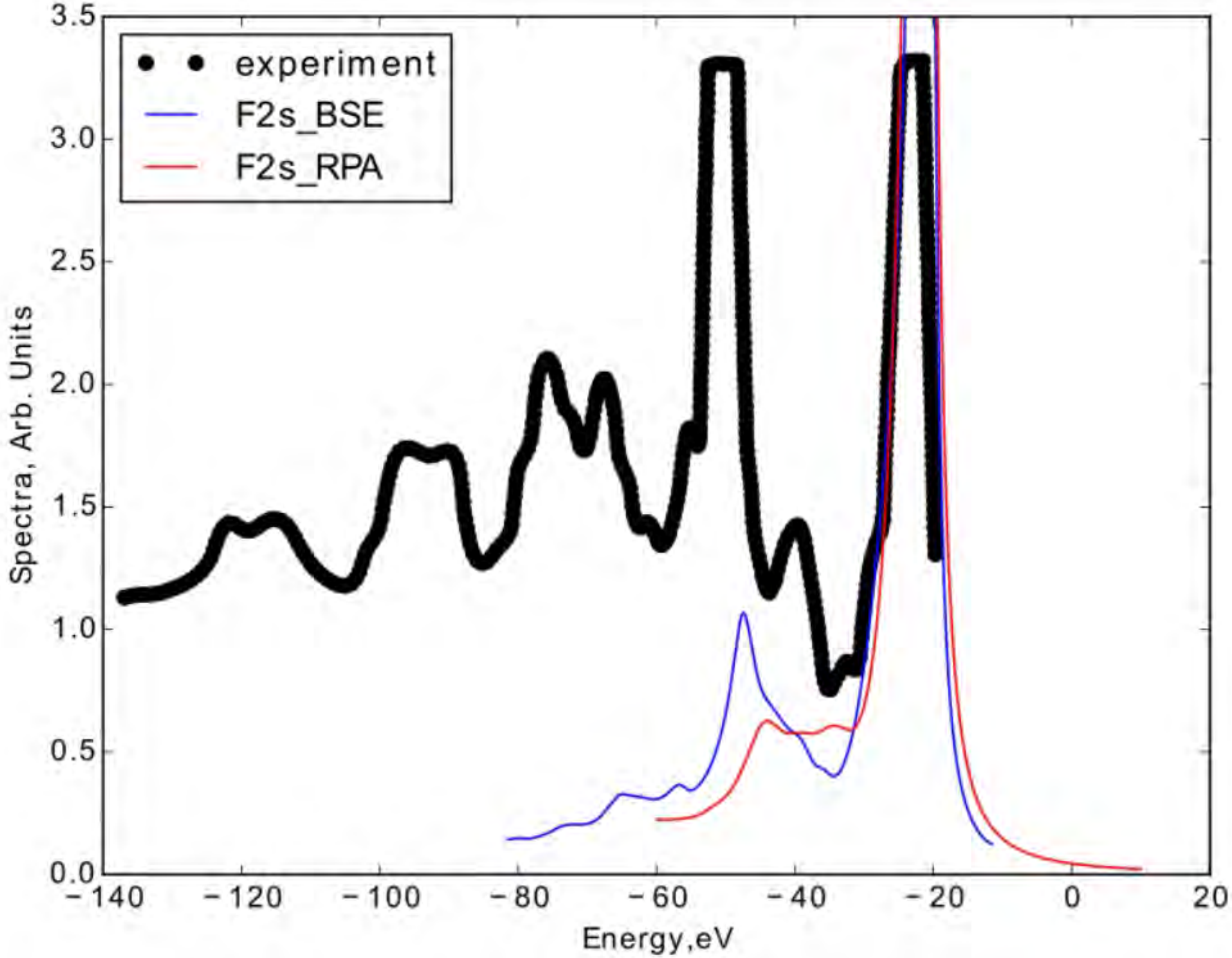
The whole matrix → follow excitations in real space and time

Consequences of excitons?

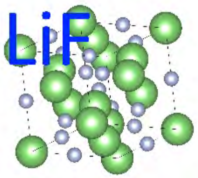
PhD thesis I. Reshetnyak

Excitonic effects in photoemission satellites

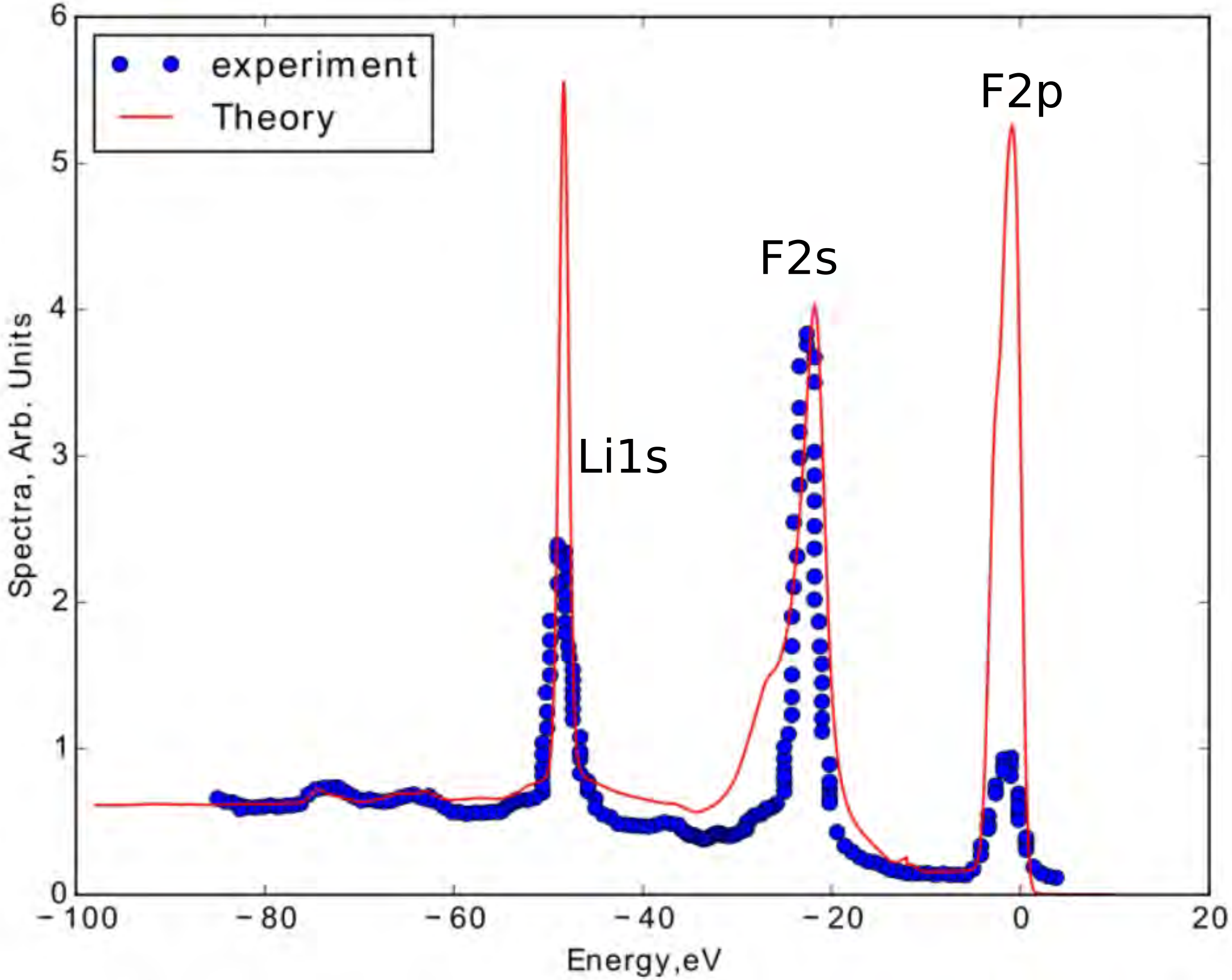




[1] Marisa Scrocco Phys. Rev. B, 1985.

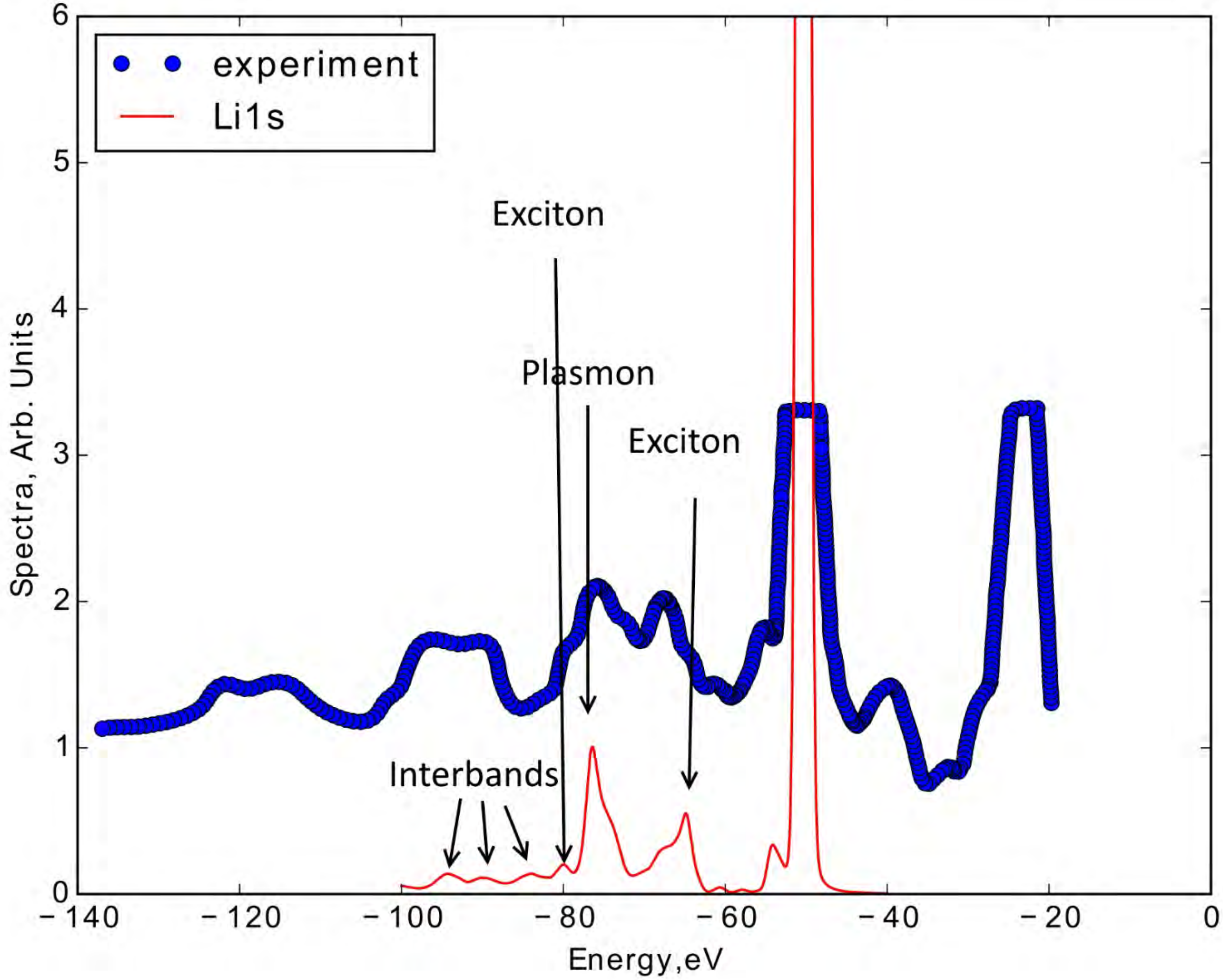


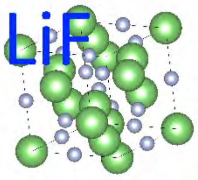
Overall comparison to experiments



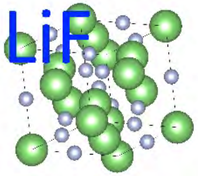
[1] S. P. Kowalczyk et al. *Phys. Rev. B*, 1974

Analysis

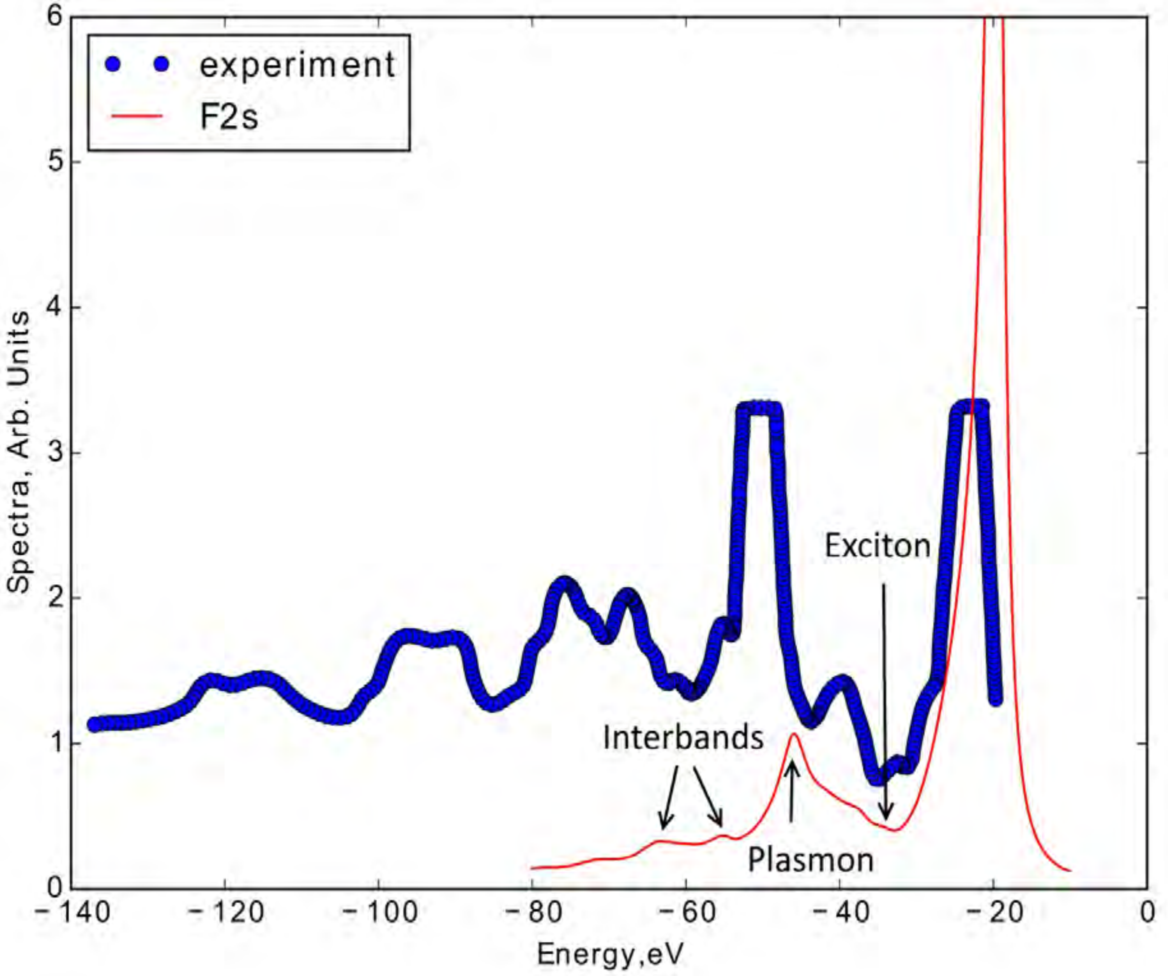




[1] Marisa Scrocco Phys. Rev. B, 1985.



Analysis



[1] Marisa Scrocco Phys. Rev. B, 1985.

The Bethe-Salpeter Equation

→ Concepts

→ TD-GFT

→ The electron-hole problem

→ Approximations

→ Realizations

→ Applications

→ Notes

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
New book containing many-body perturbation theory, DMFT and QMC

http://etsf.polytechnique.fr