Time Dependent Density Functional Theory

Lucia Reining & Francesco Sottile
Palaiseau Theoretical Spectroscopy Group

Time Dependent Density Functional Theory

→ Why bother?

→ Intuitive

→ More formally

→ Approximations

→ Realizations

→ Applications

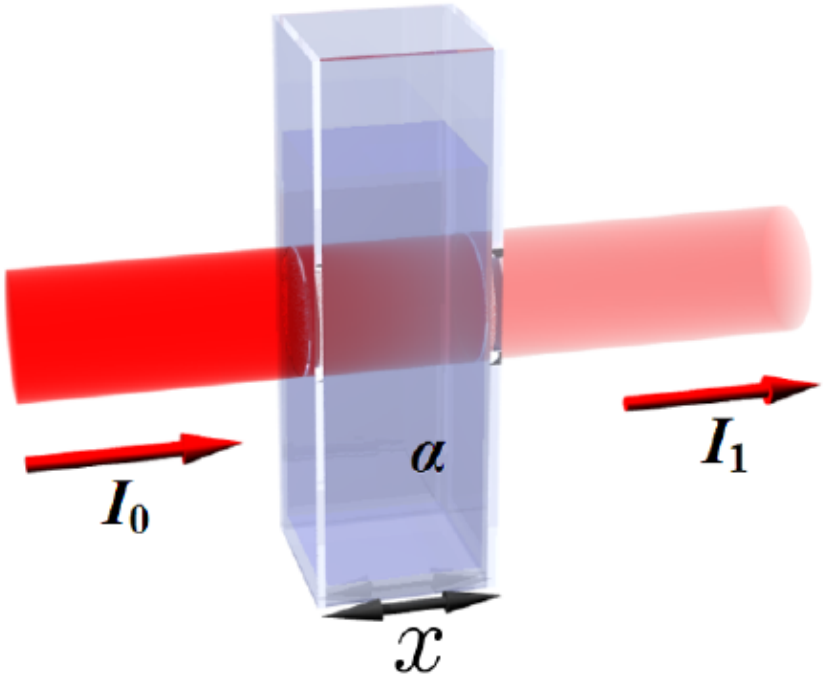
→ Notes

→ Theoretical Spectroscopy: aims and observations

Large field of research concerned with
many-electron systems in time-dependent fields

Different Phenomena

- absorption spectra
- energy loss spectra
- photo-ionization
- high-harmonic generation
- photo-emission



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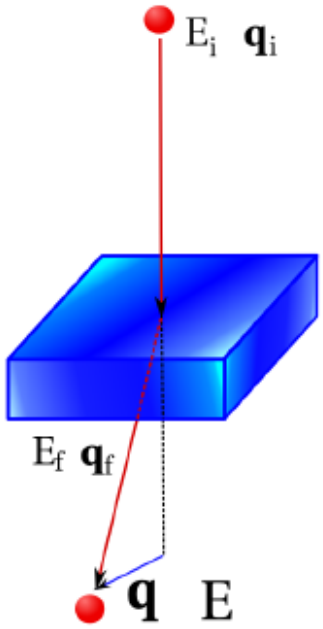

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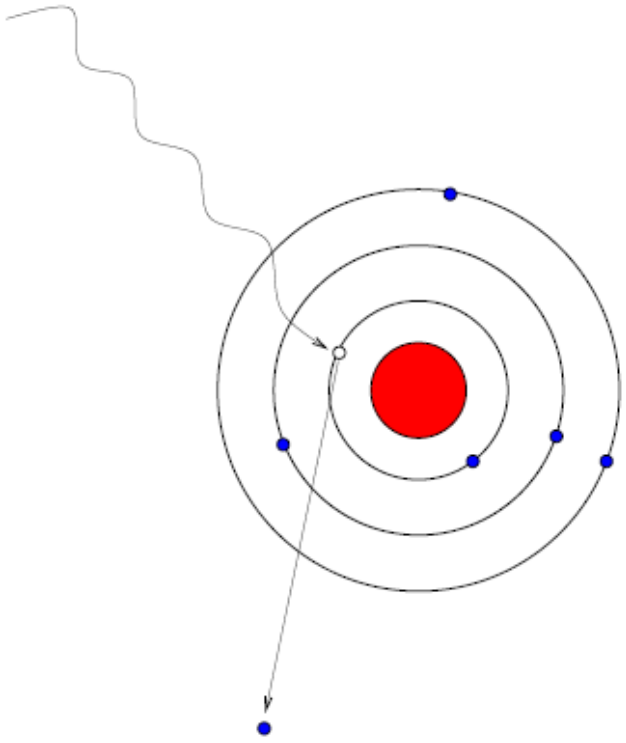

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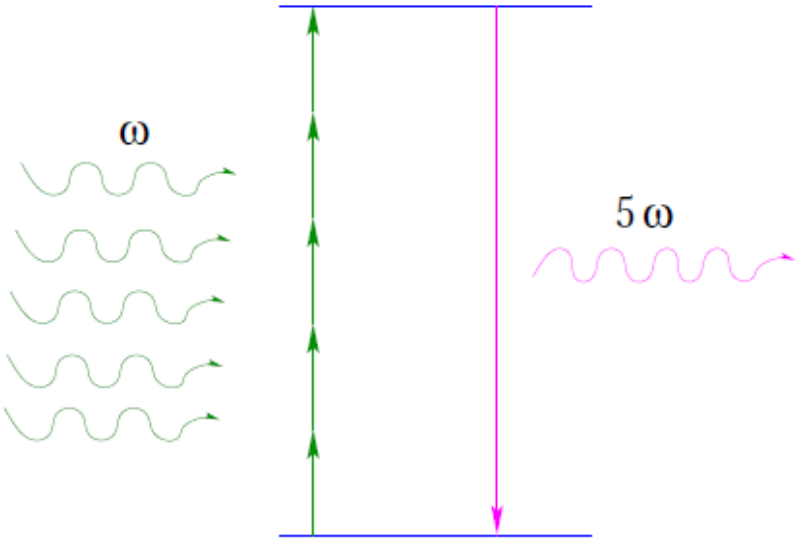

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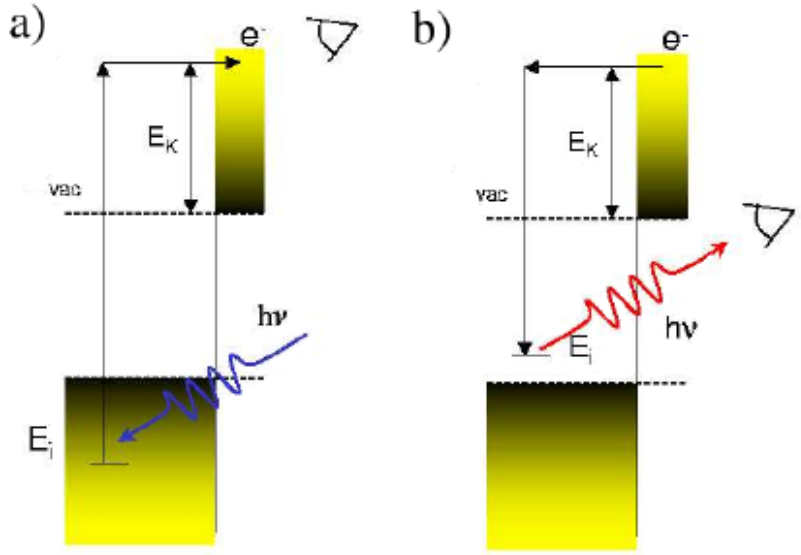


Moreover : Many-Body Perturbation Theory is dynamic !

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

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

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

$$[z - H]\, G^{tot} = I,$$

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

$$G_S(z) = \left(z - H_S - H_{SR}[z - H_R]^{-1} H_{RS}\right)^{-1} = \left([G_S^0(z)]^{-1} - H_{SR}[G_R^0(z)]H_{RS}\right)^{-1},$$

$$G_S^0 = (z - H_S)^{-1} \qquad G_R^0 = (z - H_R)^{-1}$$

$$G_S(z) = \left([G_S^0(z)]^{-1} - \Sigma(z)\right)^{-1}$$

$$\Sigma(z) = [G_S^0(z)]^{-1} - [G_S(z)]^{-1} = H_{SR}[G_R^0(z)]H_{RS}.$$

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

→ Theoretical Spectroscopy: aims and observations

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

?

→ 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

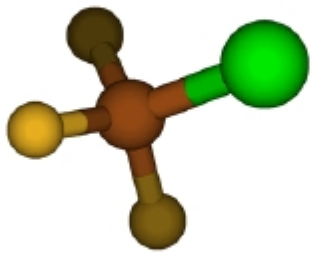
$$V_{tot}(\omega) = \varepsilon^{-1}(\omega) V_{ext}(\omega)$$

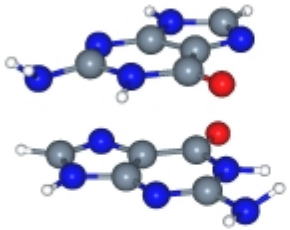
Do not want: → *all many-body* $\psi_n(x_1,....x_N)$

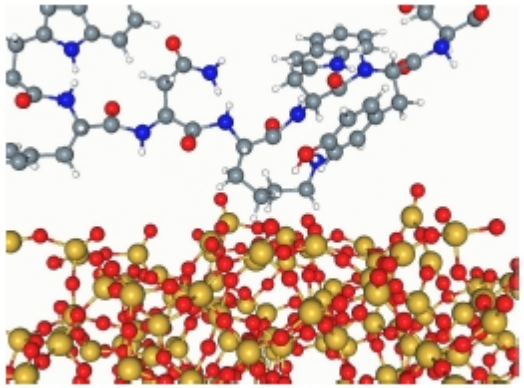
→ The effective quantities:

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

CI, QMC	GF methods (GW, BSE)	DF







→ The effective world:

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

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

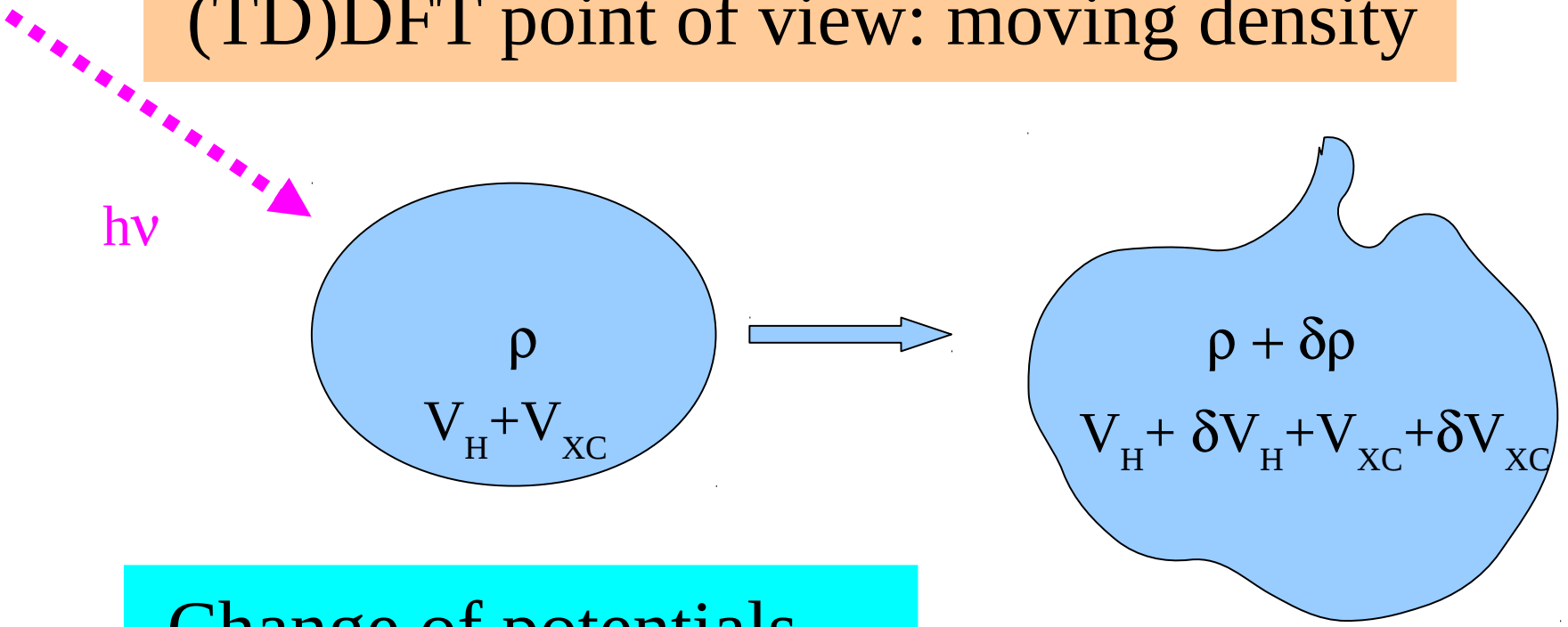
→ Theoretical Spectroscopy: tools

Effective quantities in an effective world

Time-dependent quantities – TD world

TDDFT intuitive :

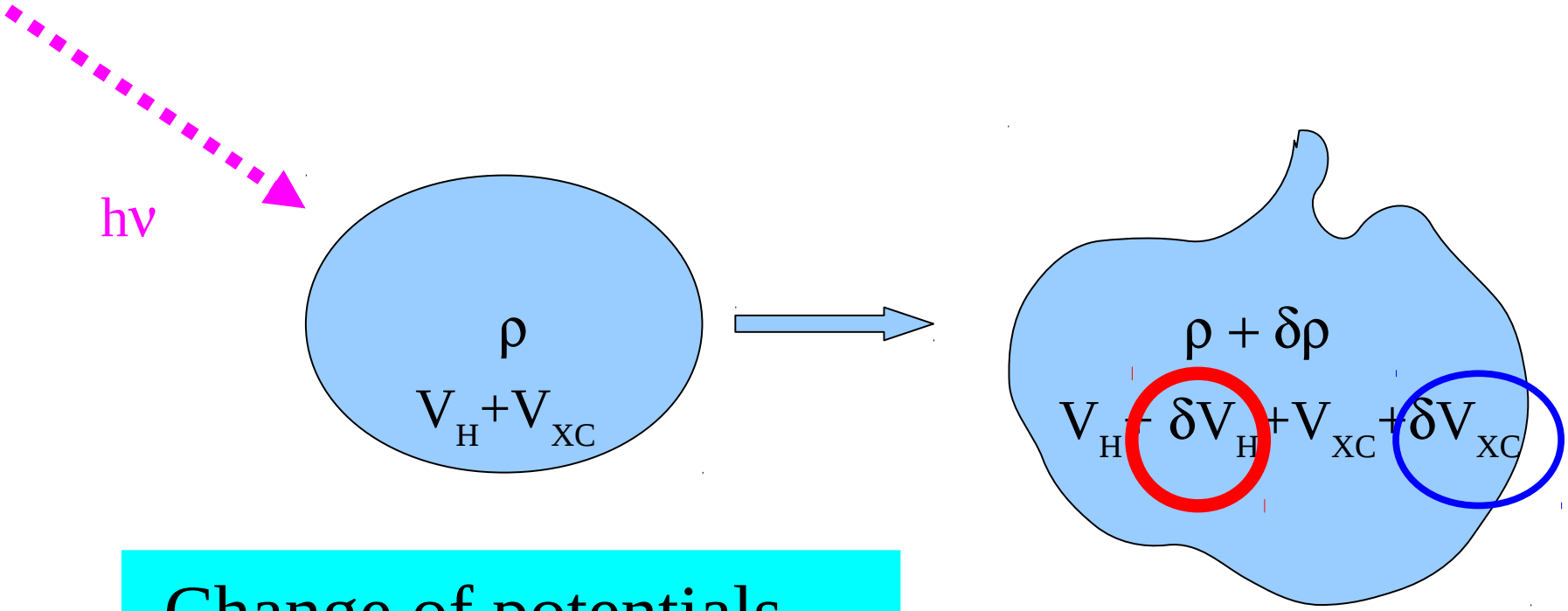
(TD)DFT point of view: moving density



Change of potentials

Excitation ?

→ Induced potentials



Change of potentials

RPA

TDLDA, ….

TDDFT formal :

DFT

Hohenberg-Kohn theorem 1

The ground-state expectation value of any physical observable of a many-electrons system is a unique functional of the electron density $n(\mathbf{r})$

$$\langle \varphi^0 | \, \widehat{O} \, | \varphi^0 \rangle = O[n]$$

P. Hohenberg and W. Kohn
Phys.Rev. **136**, B864 (1964)
(Fermi, Slater)

TDDFT

Runge-Gross theorem

The expectation value of any physical time-dependent observable of a many-electrons system is a unique functional of the **time-dependent** electron density $n(\mathbf{r}, t)$ and of **the initial state** $\varphi^0 = \varphi(t = 0)$

$$\left\langle \varphi(t) | \widehat{O}(t) | \varphi(t) \right\rangle = O[n, \varphi^0](t)$$

E. Runge and E.K.U. Gross
Phys.Rev.Lett. **52**, 997 (1984)
(Ando,Zangwill and Soven)

DFT

Static problem

Second-order differential equation
Boundary-value problem.

$$H\varphi(\mathbf{r}_1, .., \mathbf{r}_N) = E\varphi(\mathbf{r}_1, .., \mathbf{r}_N)$$

TDDFT

Time-dependent problem

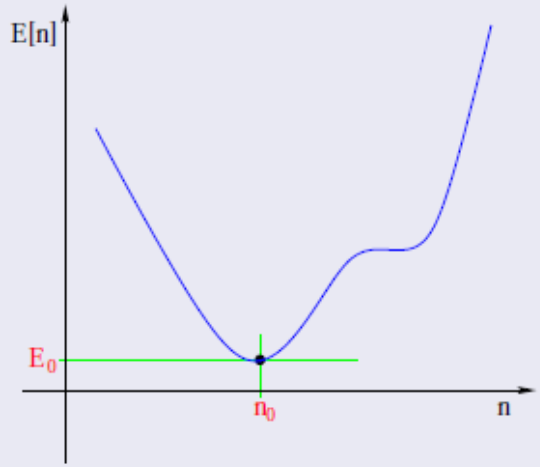
First-order differential equation
Initial-value problem

$$H(t)\varphi(\mathbf{r}_1, .., \mathbf{r}_N; t) = \imath\hbar\frac{\partial}{\partial t}\varphi(\mathbf{r}_1, .., \mathbf{r}_N; t)$$

DFT

Hohenberg-Kohn theorem 2

The total energy functional has a minimum, the ground-state energy E_0, corresponding to the ground-state density n_0.

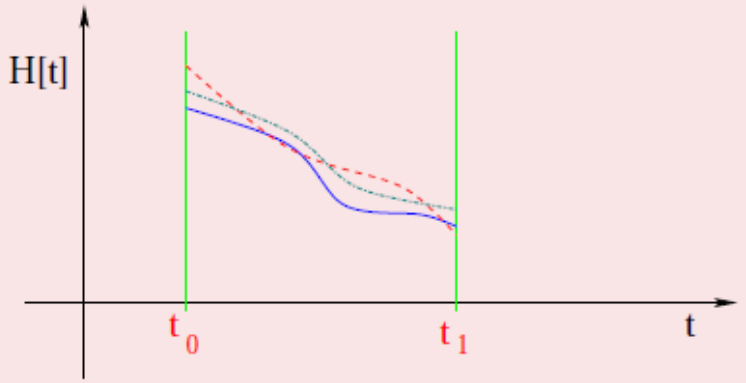


TDDFT

Runge-Gross theorem - No minimum

Time-dependent Schrödinger eq. (initial condition $\varphi(t=0)=\varphi_0$), corresponds to a **stationary** point of the Hamiltonian action

$$A = \int_{t_0}^{t_1} dt \, \langle \varphi(t) | \, \imath \frac{\partial}{\partial t} - H(t) \, | \varphi(t) \rangle$$



DFT

Kohn-Sham equations

$$\left[-\frac{1}{2}\cdot\nabla_i^2 + V_{tot}(\mathbf{r})\right]\phi_i(\mathbf{r}) = \epsilon_i\phi_i(\mathbf{r})$$

$$V_{tot}(\mathbf{r}) = V_{ext}(\mathbf{r}) + \int d\mathbf{r}'\, v(\mathbf{r},\mathbf{r}')n(\mathbf{r}') + V_{xc}\left([n],\mathbf{r}\right)$$

$$V_{xc}\left([n],\mathbf{r}\right) = \frac{\delta E_{xc}[n]}{\delta n(\mathbf{r})}$$

Unknown exchange-correlation potential.
V_{xc} functional of the density.

TDDFT

Time-dependent Kohn-Sham equations

$$\left[-\frac{1}{2}\nabla^2 + V_{tot}(\mathbf{r},t)\right]\phi_i(\mathbf{r},t) = i\frac{\partial}{\partial t}\phi_i(\mathbf{r},t)$$

$$V_{tot}(\mathbf{r},t) = V_{ext}(\mathbf{r},t) + \int v(\mathbf{r},\mathbf{r}')n(\mathbf{r}',t)d\mathbf{r}' + V_{xc}([n]\mathbf{r},t)$$

$$V_{xc}\left([n],\mathbf{r},t\right) = \frac{\delta A_{xc}[n]}{\delta n(\mathbf{r},t)}$$

Unknown exchange-correlation time-dependent potential.
V_{xc} functional of the density **at all times** and of the **initial state**.

Demonstrations, further readings, etc.

R. van Leeuwen
Int.J.Mod.Phys. **B15**, 1969 (2001)

$$V_{xc}\left([n],\mathbf{r},t\right)=\frac{\delta A_{xc}[n]}{\delta n(\mathbf{r},t)}$$

$$\frac{\delta V_{xc}\left([n],\mathbf{r},t\right)}{\delta n(\mathbf{r}',t')}=\frac{\delta^2 A_{xc}[n]}{\delta n(\mathbf{r},t)\delta n(\mathbf{r}',t')}$$

Causality-Symmetry dilemma

DFT

Hohenberg-Kohn theorem

The ground-state expectation value of any physical observable of a many-electrons system is a unique functional of the electron density $n(\mathbf{r})$

$$\left\langle \varphi^0 \middle| \widehat{O} \middle| \varphi^0 \right\rangle = O[n]$$

Kohn-Sham equations

$$\left[-\frac{1}{2}\nabla_i^2 + V_{tot}(\mathbf{r}) \right] \phi_i(\mathbf{r}) = \epsilon_i \phi_i(\mathbf{r})$$

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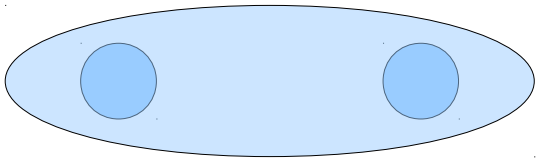
$$\left[-\frac{1}{2}\nabla^2 + V_{tot}(\mathbf{r}, t) \right] \phi_i(\mathbf{r}, t) = i\frac{\partial}{\partial t}\phi_i(\mathbf{r}, t)$$

Approximations

The problem: $V_{xc}[n](r)$ *means* $V_{xc}(n(r_1,r_2,....r_N),r)$

Reason: * the Coulomb interaction

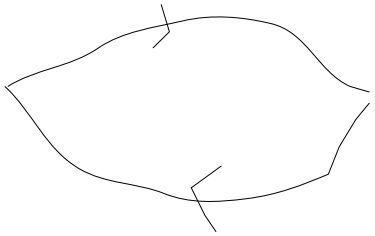
* hybridization



The problem: $V_{xc}[n](r,t)$ *means* $V_{xc}(n(r_1,r_2,....r_{N;}\ t_1.....t_n),r,t)$

Reason: * the Coulomb interaction

* polarization



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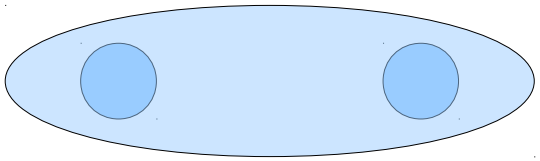
* hybridization 

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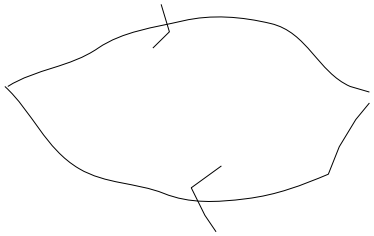
* polarization 

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"Solution": LDA $V_{xc}(n(r),r)$, from HEG

The problem: $V_{xc}[n](r,t)$ *means* $V_{xc}(n(r_1,r_2,....r_{N;}\, t_1.....t_n),r,t)$

"Solution": ALDA $V_{xc}(n(r,t),r,t)$, from HEG

Realizations

First Approach: Time Evolution of KS equations

$$[H_{KS}(t)]\,\phi_i(\mathbf{r},t) = i\frac{\partial}{\partial t}\phi_i(\mathbf{r},t)$$

$$n(\mathbf{r},t) = \sum_i^{occ} |\phi_i(\mathbf{r},t)|^2$$

$$\phi(t) = \hat{U}(t,t_0)\phi(t_0)$$

$$U(t,t_0) = 1 - i\int_{t_0}^{t} d\tau H(\tau)\hat{U}(\tau,t_0)$$

A. Castro *et al.* J.Chem.Phys. **121**, 3425 (2004)

Photo-absorption cross section σ

$$\sigma(\omega) = \frac{4\pi\omega}{c}\mathrm{Im}\alpha(\omega)$$

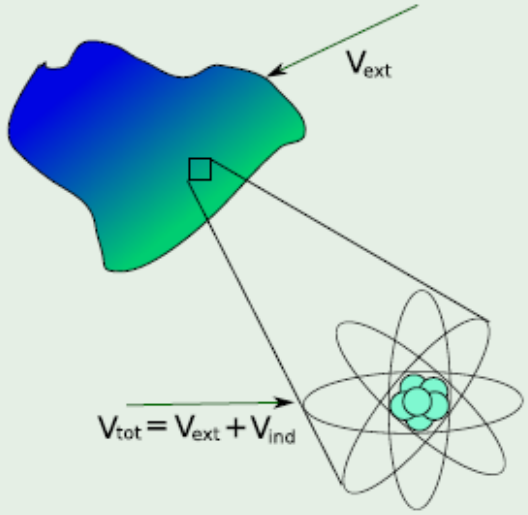
$$\alpha(t) = -\int d\mathbf{r}\, V_{ext}(\mathbf{r}, t) n(\mathbf{r}, t)$$

in dipole approximation ($\lambda \ggg$ dimension of the system)

$$\sigma_{zz}(\omega) = -\frac{4\pi\omega}{c}\mathrm{Im}\ \alpha(\omega) = -\frac{4\pi\omega}{\mathrm{c}}\mathrm{Im}\int \mathrm{d}\mathbf{r}\ \mathrm{z}\ \mathrm{n}(\mathbf{r}, \omega)$$

Linear Response Approach

System submitted to an external perturbation

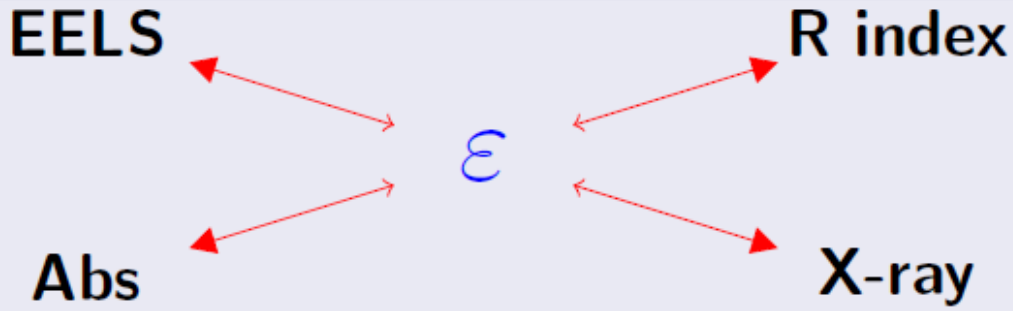


$$V_{tot} = \varepsilon^{-1} V_{ext}$$

$$V_{tot} = V_{ext} + V_{ind}$$

$$\mathbf{E} = \varepsilon^{-1} \mathbf{D}$$

Dielectric function ε



Definition of polarizability

$$\begin{aligned} \text{not polarizable} &\Rightarrow V_{tot} = V_{ext} \Rightarrow \varepsilon^{-1} = 1 \\ \text{polarizable} &\Rightarrow V_{tot} \neq V_{ext} \Rightarrow \varepsilon^{-1} \neq 1 \\ & \qquad\qquad\quad\; \varepsilon^{-1} = 1 + v\chi \end{aligned}$$

χ is the polarizability of the system

Polarizability

interacting system $\delta n = \chi \delta V_{ext}$

non-interacting system $\delta n_{n-i} = \chi^0 \delta V_{tot}$

Single-particle polarizability

$$\chi^0 = \sum_{ij} \frac{\phi_i(\mathbf{r})\phi_j^*(\mathbf{r})\phi_i^*(\mathbf{r}')\phi_j(\mathbf{r}')}{\omega - (\epsilon_i - \epsilon_j)}$$

hartree, hartree-fock, dft, etc.

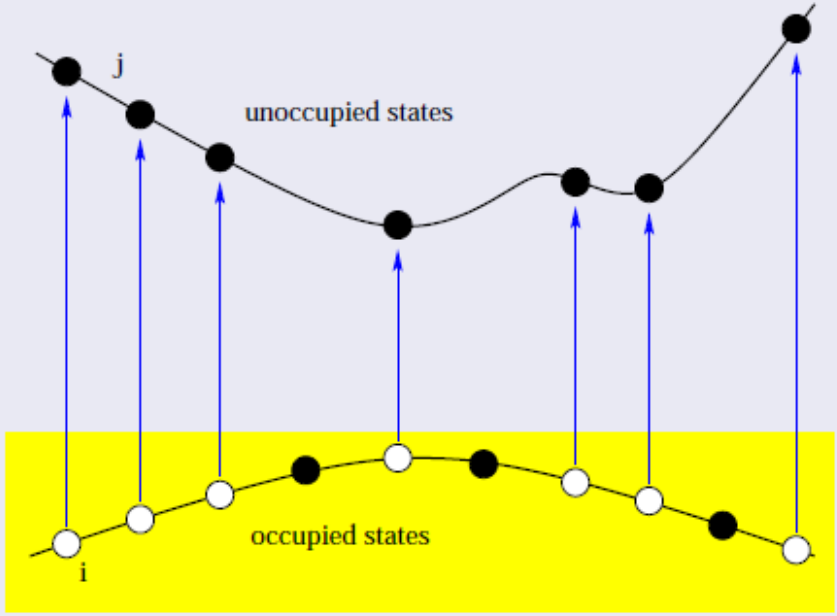
G.D. Mahan *Many Particle Physics* (Plenum, New York, 1990)

Polarizability

interacting system $\delta n = \chi \delta V_{ext}$

non-interacting system $\delta n_{n-i} = \chi^0 \delta V_{tot}$

$$\chi^0 = \sum_{ij} \frac{\phi_i(\mathbf{r})\phi_j^*(\mathbf{r})\phi_i^*(\mathbf{r}')\phi_j(\mathbf{r}')}{\omega - (\epsilon_i - \epsilon_j)}$$



Polarizability

$$\chi \delta V_{ext} = \chi^0 \left(\delta V_{ext} + \delta V_H + \delta V_{xc} \right)$$

$$\chi = \chi^0 \left(1 + \frac{\delta V_H}{\delta V_{ext}} + \frac{\delta V_{xc}}{\delta V_{ext}} \right)$$

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

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

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

with f_{xc} = exchange-correlation kernel

Polarizability

$$\chi \delta V_{ext} = \chi^0 \left(\delta V_{ext} + \delta V_H + \delta V_{xc} \right)$$

$$\chi = \chi^0 \left(1 + \frac{\delta V_H}{\delta V_{ext}} + \frac{\delta V_{xc}}{\delta V_{ext}} \right)$$

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

$$\chi = \left[1 - \chi^0 \left(v + f_{xc} \right) \right]^{-1} \chi^0$$

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

Polarizability χ in TDDFT

1. DFT ground-state calc. $\rightarrow$ ϕ_i, ϵ_i $[V_{xc}]$
2. $\phi_i, \epsilon_i \rightarrow \chi^0 = \sum_{ij} \frac{\phi_i(\mathbf{r})\phi_j^*(\mathbf{r})\phi_i^*(\mathbf{r}')\phi_j(\mathbf{r}')}{\omega-(\epsilon_i-\epsilon_j)}$
3. $\left.\begin{array}{l} \frac{\delta V_H}{\delta n} = v \\ \frac{\delta V_{xc}}{\delta n} = f_{xc} \end{array}\right\}$ variation of the potentials
4. $\chi = \chi^0 + \chi^0 (v + f_{xc}) \chi$ $\quad f_{xc}(r,r',t-t') \rightarrow f_{xc}(r,r',\omega)$

A comment

- $f_{xc} = \begin{cases} \frac{\delta V_{xc}}{\delta n} \\ \text{“any” other function} \end{cases}$

Reciprocal space

$$\chi^0_{GG'}(\mathbf{q},\omega) = \sum_{vc\mathbf{k}} \frac{\left\langle \phi_{v\mathbf{k}} \middle| e^{\imath(\mathbf{q}+\mathbf{G})\mathbf{r}} \middle| \phi^*_{c\mathbf{k}+\mathbf{q}} \right\rangle \left\langle \phi_{c\mathbf{k}+\mathbf{q}} \middle| e^{-\imath(\mathbf{q}+\mathbf{G}')\mathbf{r}'} \middle| \phi^*_{v\mathbf{k}} \right\rangle}{\omega - \left(\epsilon_{c\mathbf{k}+\mathbf{q}} - \epsilon_{v\mathbf{k}}\right) + \imath\eta}$$

$$\chi_{GG'}(\mathbf{q},\omega) = \chi^0 + \chi^0 \left(v + f_{xc}\right) \chi$$

$$\varepsilon^{-1}_{GG'}(\mathbf{q},\omega) = \delta_{GG'} + v_G(\mathbf{q}) \chi_{GG'}(\mathbf{q},\omega)$$

$$\mathrm{ELS}(\mathbf{q},\omega) = -\mathrm{Im}\left\{\varepsilon^{-1}_{00}(\mathbf{q},\omega)\right\} \;;\; \mathrm{Abs}(\omega) = \lim_{\mathbf{q}\to 0} \mathrm{Im}\left\{\frac{1}{\varepsilon^{-1}_{00}(\mathbf{q},\omega)}\right\}$$

S.L.Adler, Phys.Rev **126**, 413 (1962); N.Wiser Phys.Rev **129**, 62 (1963)

Microscopic components $\bar{v}$

$$\bar{v} = \text{local field effects}$$

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

$$\text{Abs}^{\text{NLF}} = -v_0 \, \text{Im} \left\{ \bar{\chi}^{\text{NLF}} \right\}$$

$$\text{Abs}^{\text{NLF}} = \text{Im} \left\{ \varepsilon_{00} \right\}$$

$$\text{Abs} = \text{Im} \left\{ \frac{1}{\varepsilon_{00}^{-1}} \right\}$$

Practical schema and approximations

- Ground-state calculation $\rightarrow \phi_i, \epsilon_i$ [V_{xc} LDA]
- $\chi^0(\mathbf{q}, \omega)$
- $\chi = \chi^0 + \chi^0 (v + f_{xc}) \chi$

$$f_{xc} = 0 \quad \text{RPA}$$

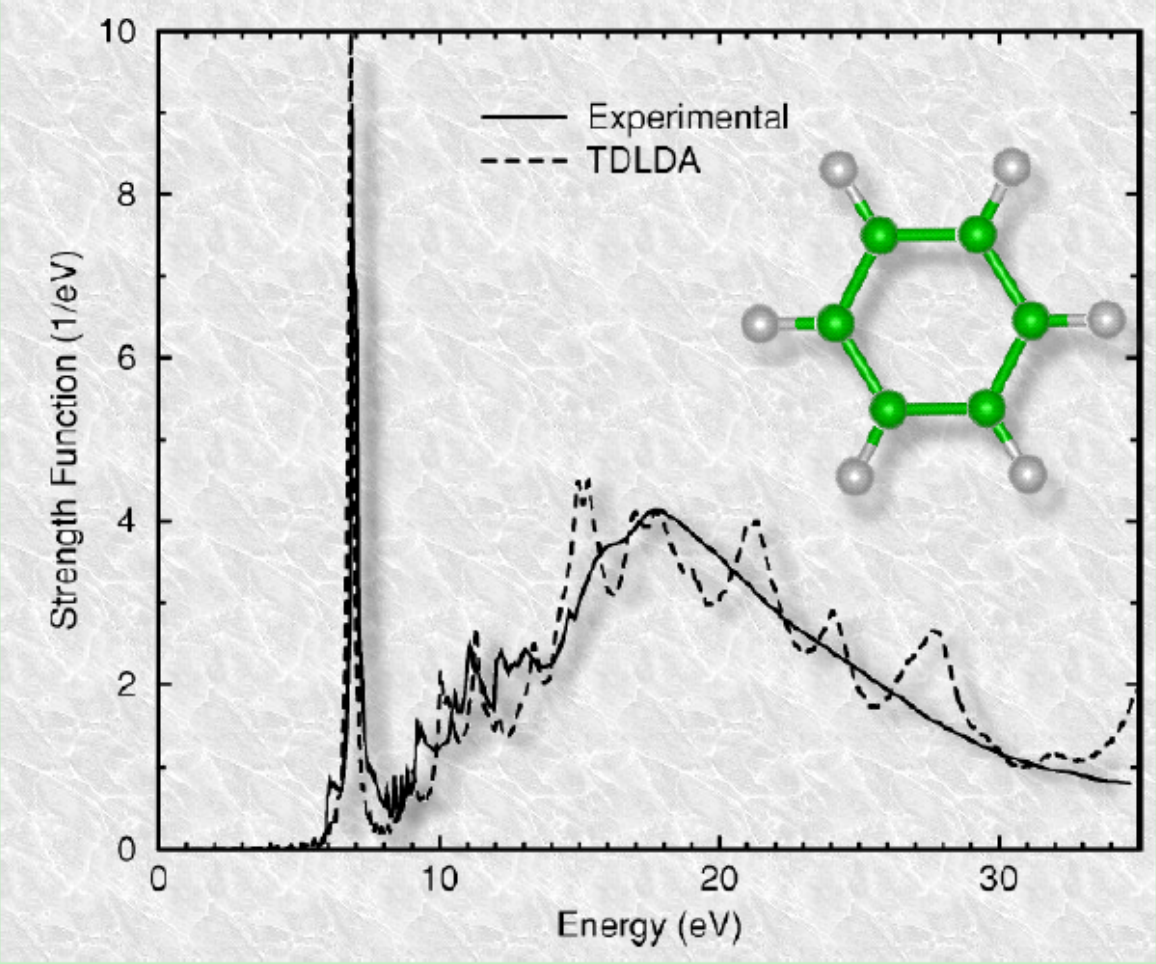
$$f_{xc}^{\text{ALDA}}(\mathbf{r}, \mathbf{r}') = \frac{\delta V_{xc}(\mathbf{r})}{\delta n(\mathbf{r}')} \delta(\mathbf{r} - \mathbf{r}') \quad \text{ALDA}$$

Applications (and what can we learn from them?)

Photo-absorption cross section of Benzene

ALDA vs EXP

$$\mathrm{Abs} = -\frac{4\pi\omega}{c}\mathrm{Im}\int \mathrm{d}\mathbf{r}\mathrm{zn}(\mathrm{r},\omega)$$



K.Yabana and G.F.Bertsch Int.J.Mod.Phys.**75**, 55 (1999)

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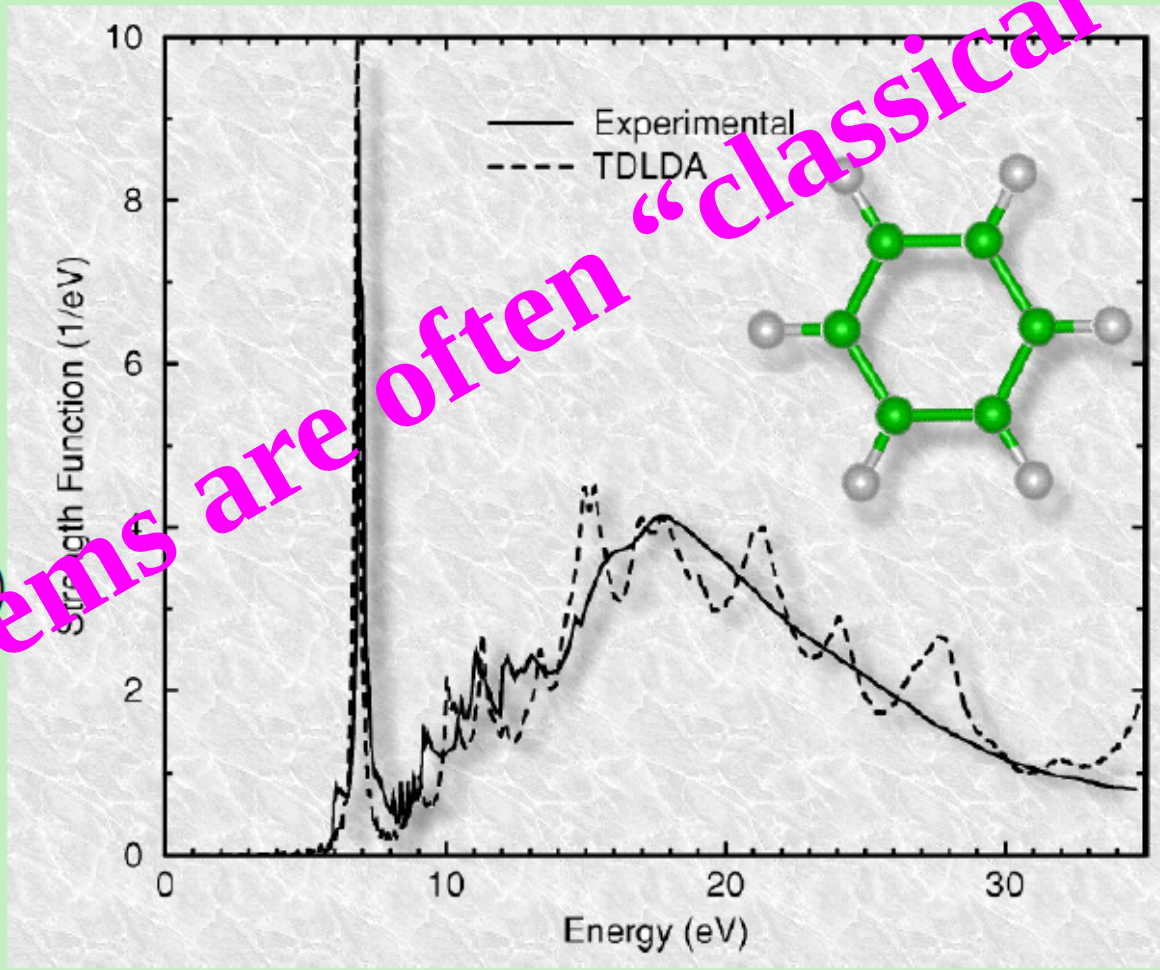
ALDA vs EXP

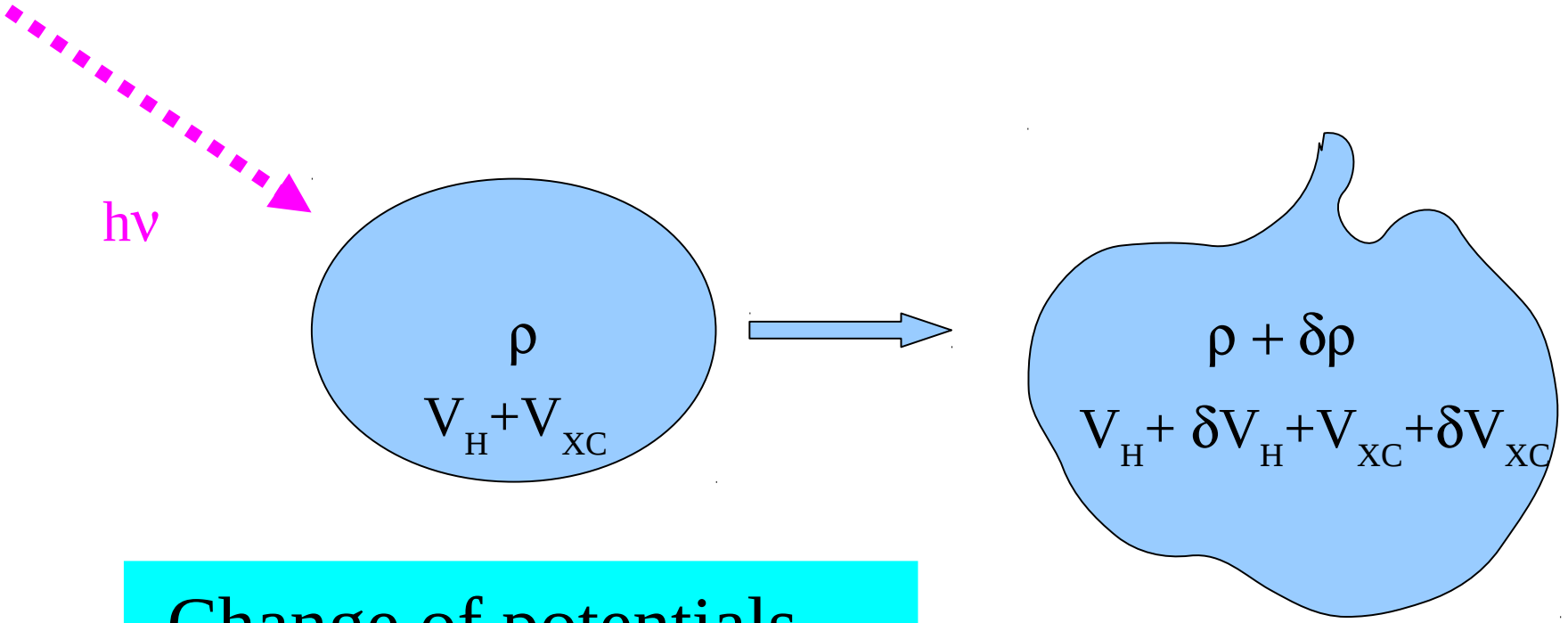
$$\mathrm{Abs} = -\frac{4\pi\omega}{c}\mathrm{Im}\int d\mathbf{r} z n(\mathrm{r},\omega)$$



Finite systems are often "classical"

K.Yabana and G.F.Bertsch Int.J.Mod.Phys.**75**, 55 (1999)

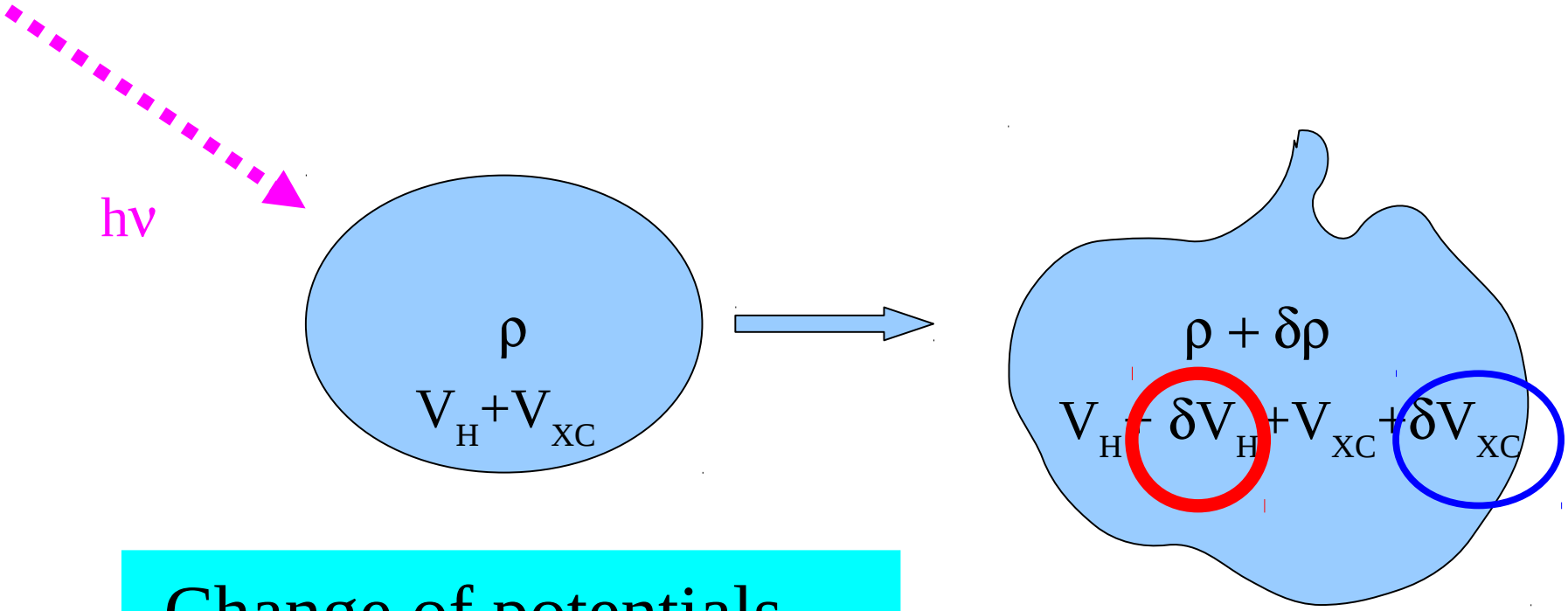
(TD)DFT point of view: moving density



Change of potentials

Excitation ?

→ Induced potentials

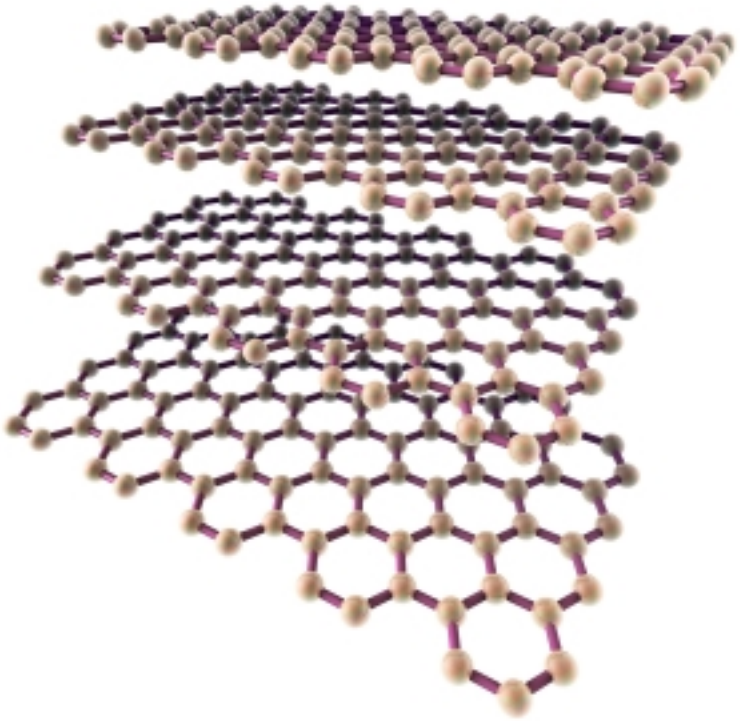


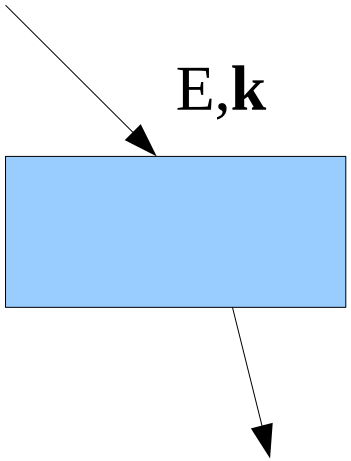
Change of potentials

RPA

TDLDA, ….

→ Interaction leads to..... coupling





Loss spectroscopy

Exp: Eberlein et al., Phys. Rev. B 77, 233406 (2008)

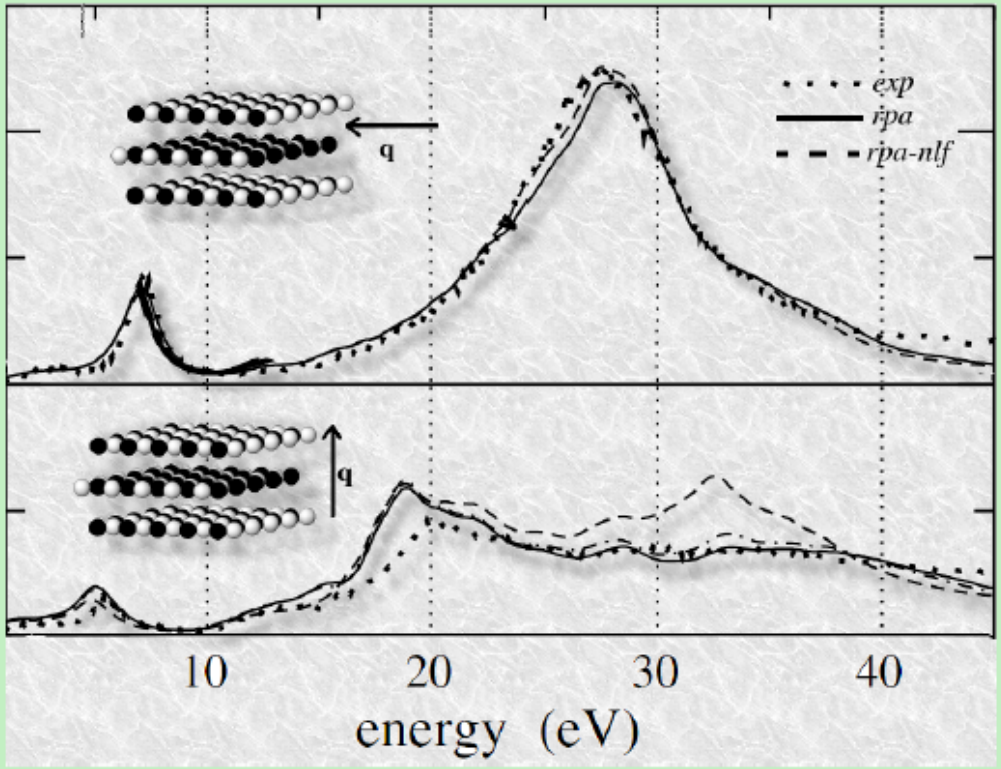
Electron Energy Loss Spectrum of Graphite

RPA vs EXP

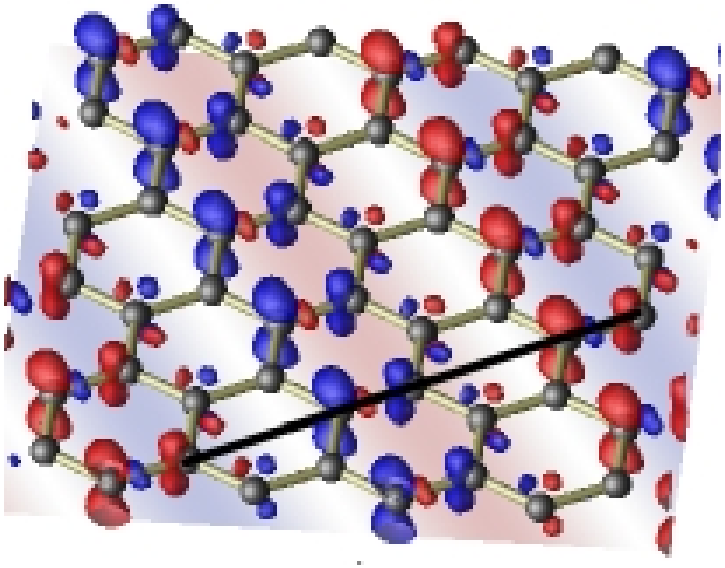
$$\chi^{NLF} = \chi^0 + \chi^0 \, v_0 \, \chi^{NLF}$$

$$\chi = \chi^0 + \chi^0 \, v \, \chi$$

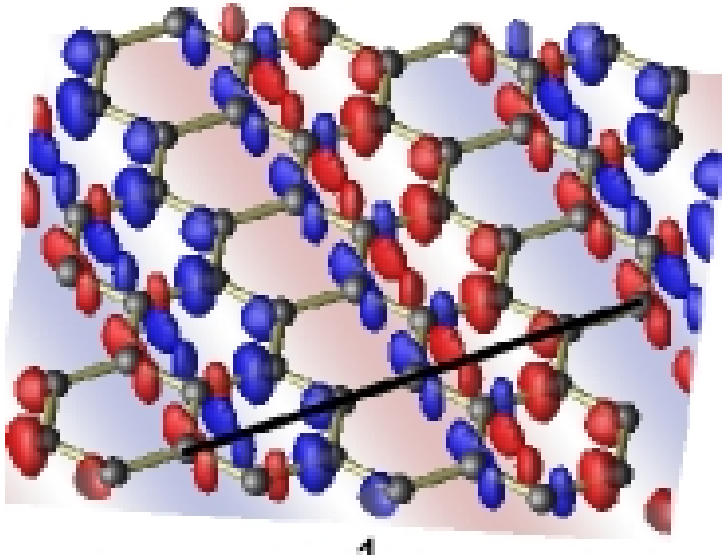
$$ELS = -v_0 \mathrm{Im}\left\{\chi_{00}\right\}$$



A.Marinopoulos *et al.* Phys.Rev.Lett **89**, 76402 (2002)



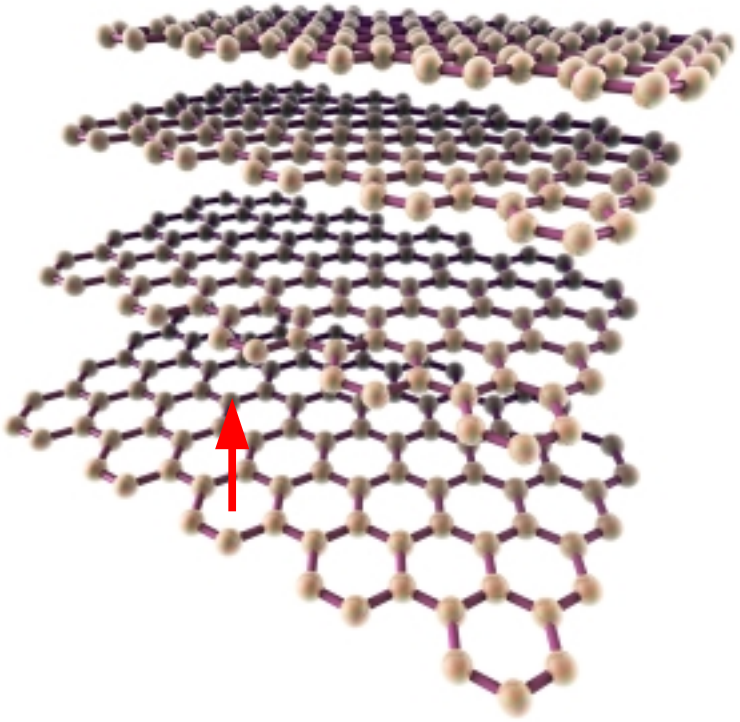
9 eV



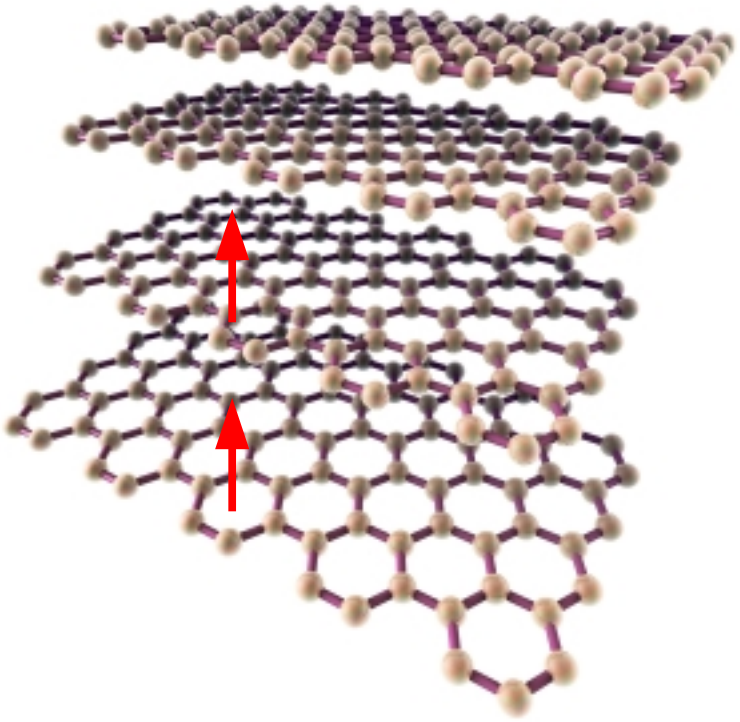
30 eV

Graphite, plasmon oscillations
(R. Hambach, PhD thesis)

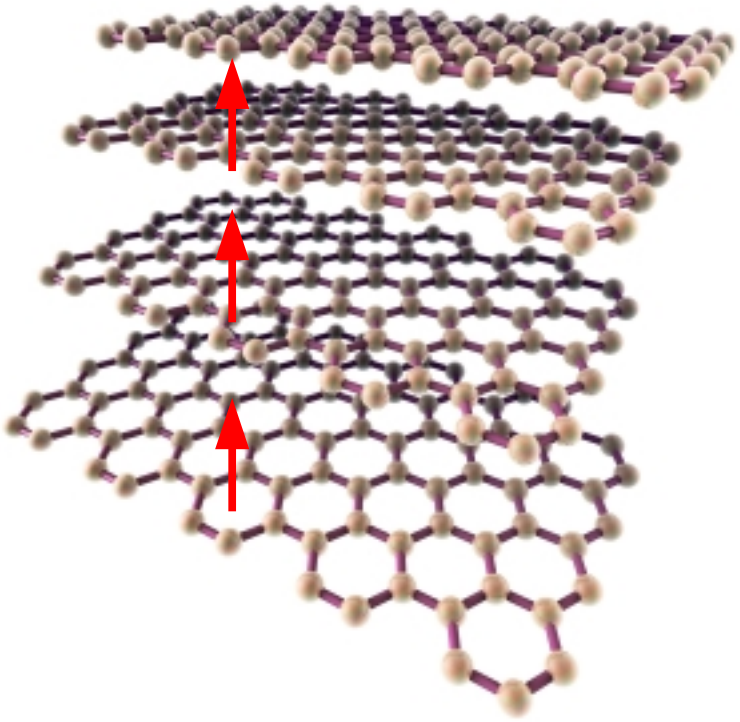
→ Interaction leads to..... coupling



→ Interaction leads to..... coupling

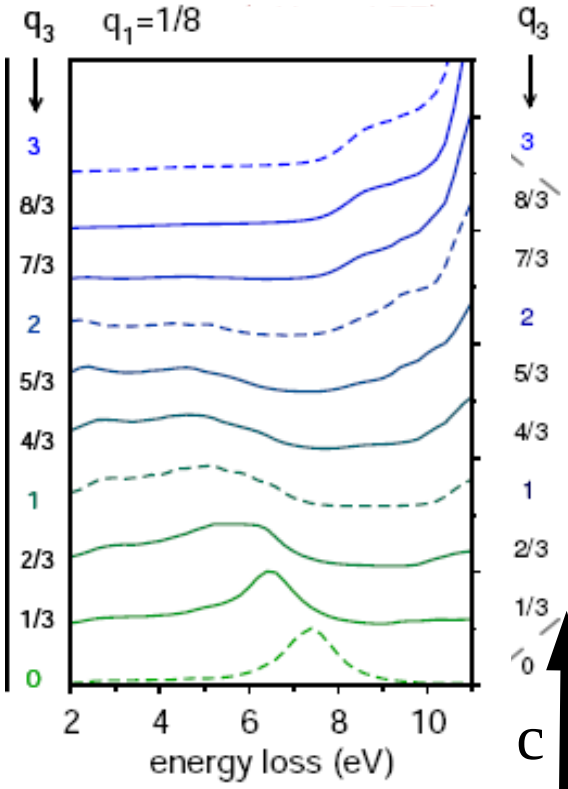


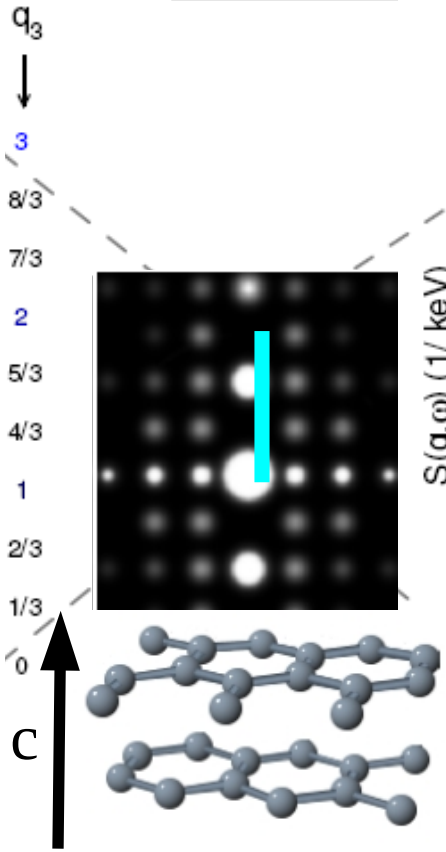
→ Interaction leads to..... coupling

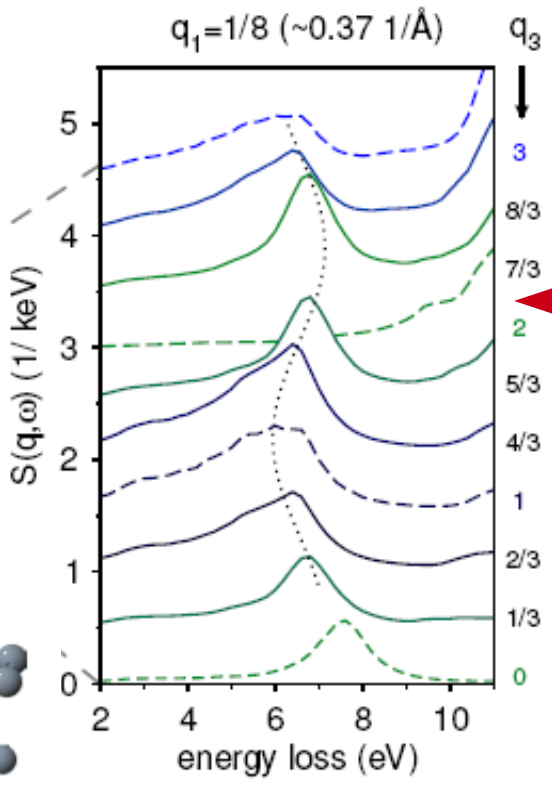


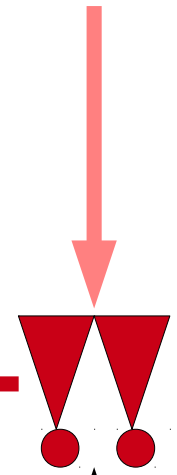
Why study this? * Unexpected effects!
* Guideline for experiments

Close to Bragg point







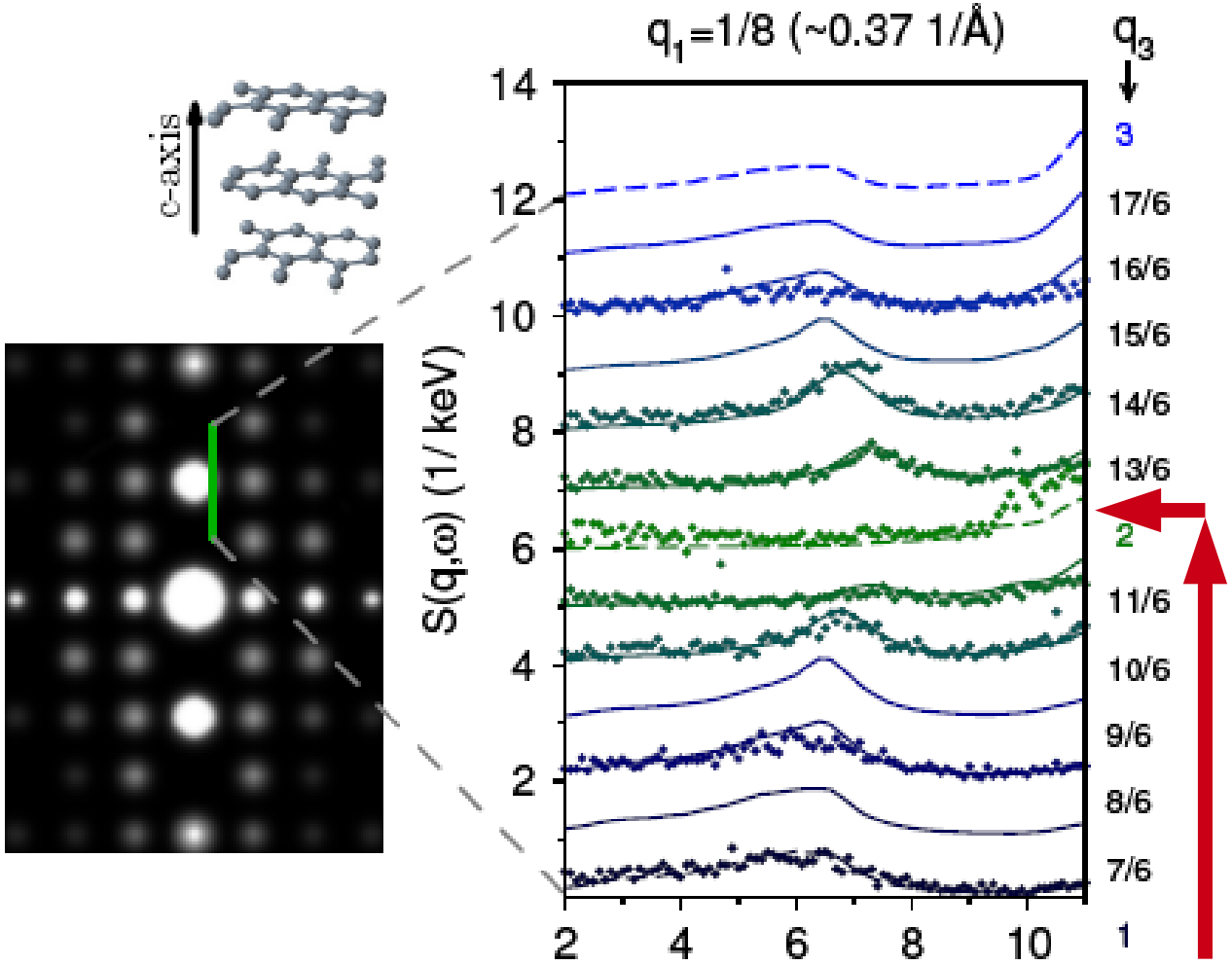


Independent particles

With induced potentials:
Induced modes

Ralf Hambach et al., Phys. Rev. Lett. **101**, 266406 (2008)

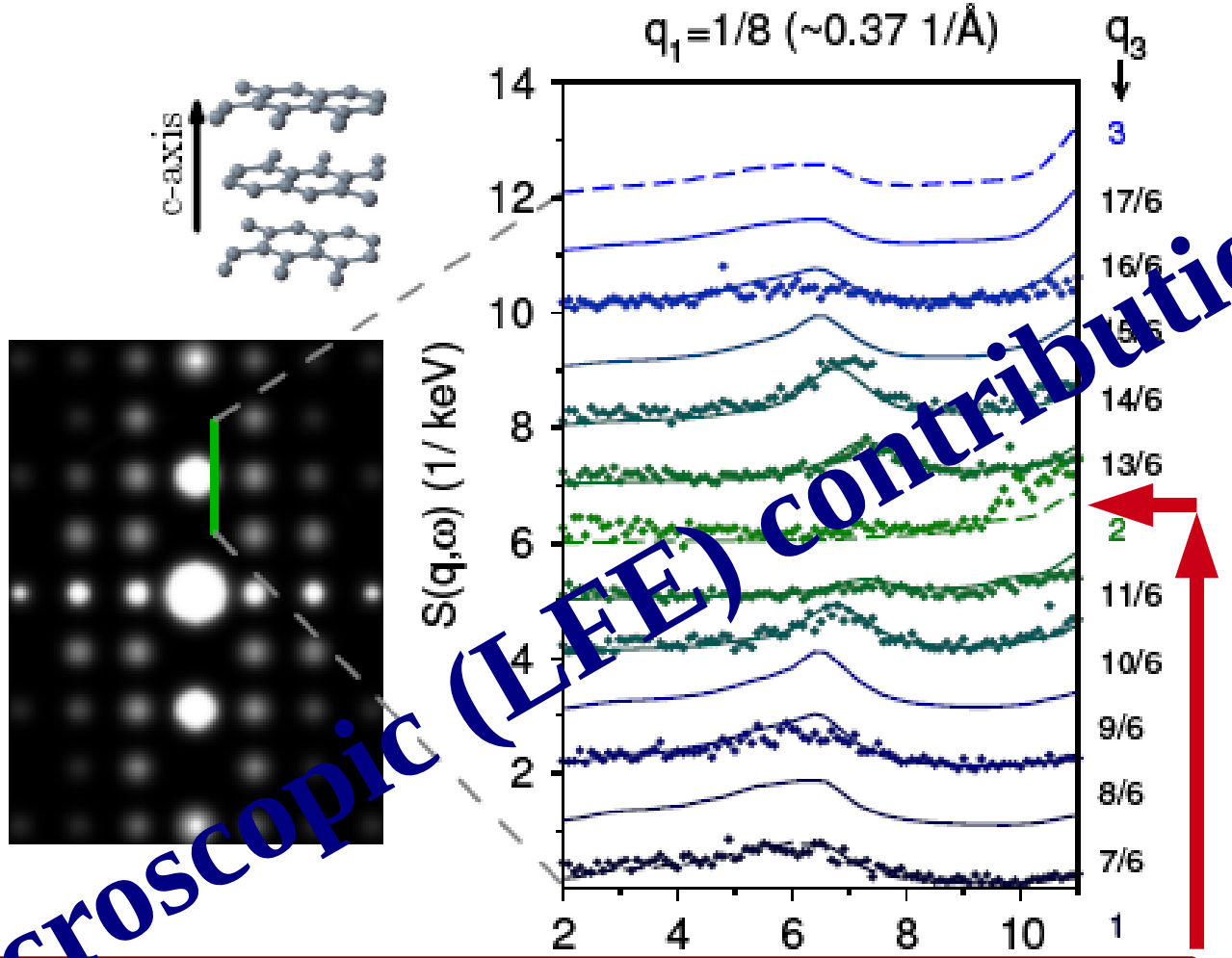
Experimental verification, N. Hiraoka et al., Spring8 Taiwan/Japan



Strong changes close to Bragg reflex!

Ralf Hambach et al., Phys. Rev. Lett. **101**, 266406 (2008)

Experimental verification, N. Hiraoka et al., Spring8 Taiwan/Japan



Microscopic (LFE) contributions!

Strong changes close to Bragg reflex!

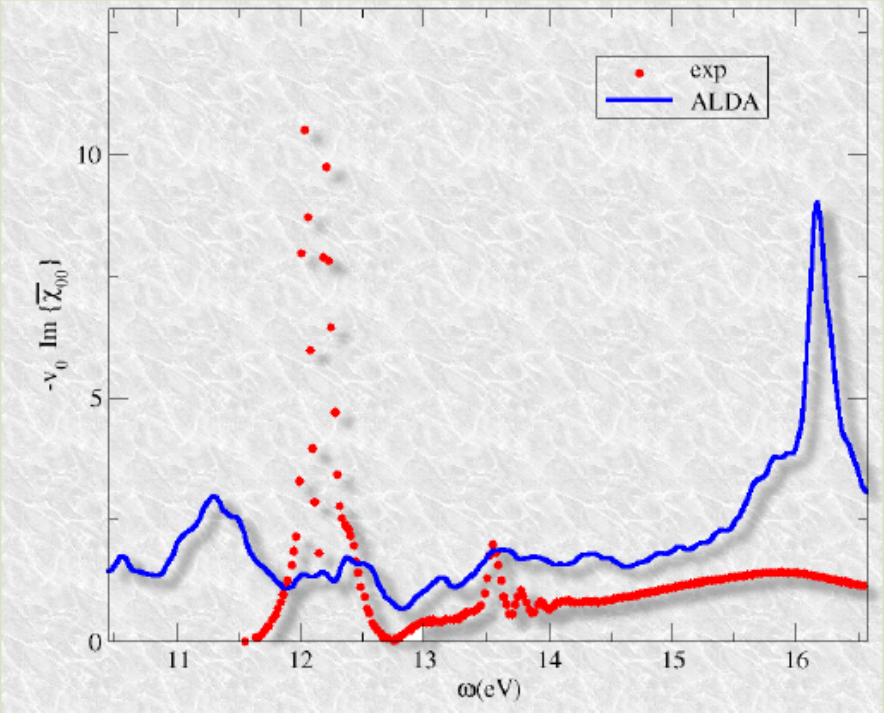
Ralf Hambach et al., Phys. Rev. Lett. **101**, 266406 (2008)

Absorption Spectrum of Argon

ALDA vs EXP

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

$$\mathsf{Abs} = -v_0 \mathrm{Im}\left\{\bar{\chi}_{00}\right\}$$



Good results

- Photo-absorption of small molecules
- ELS of solids

Bad results

- Absorption of solids

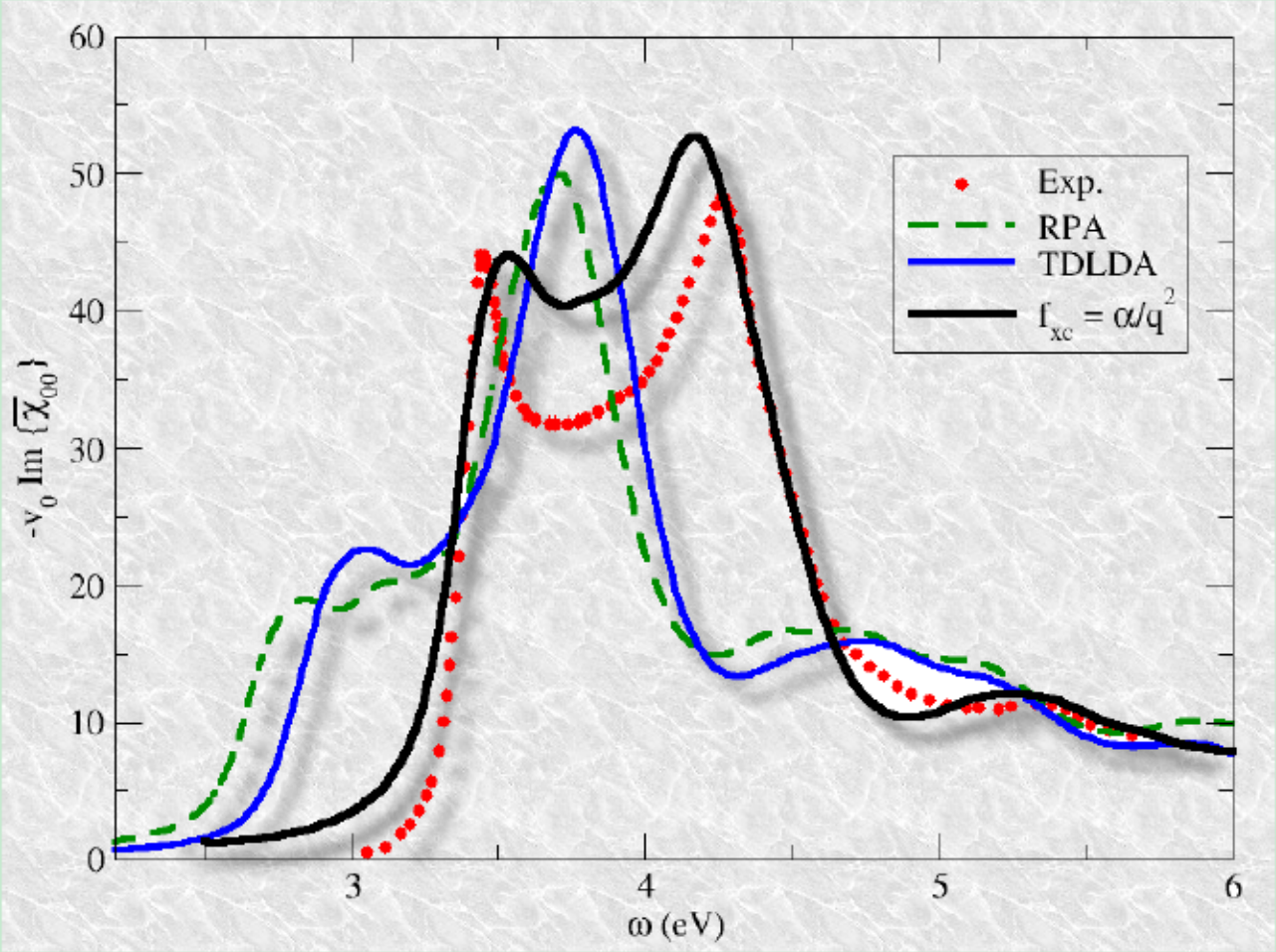
Why?

f_{xc}^{ALDA} is short-range

$$f_{xc}(\mathbf{q} \to 0) \sim \frac{1}{q^2}$$

ALDA: Achievements and Shortcomings

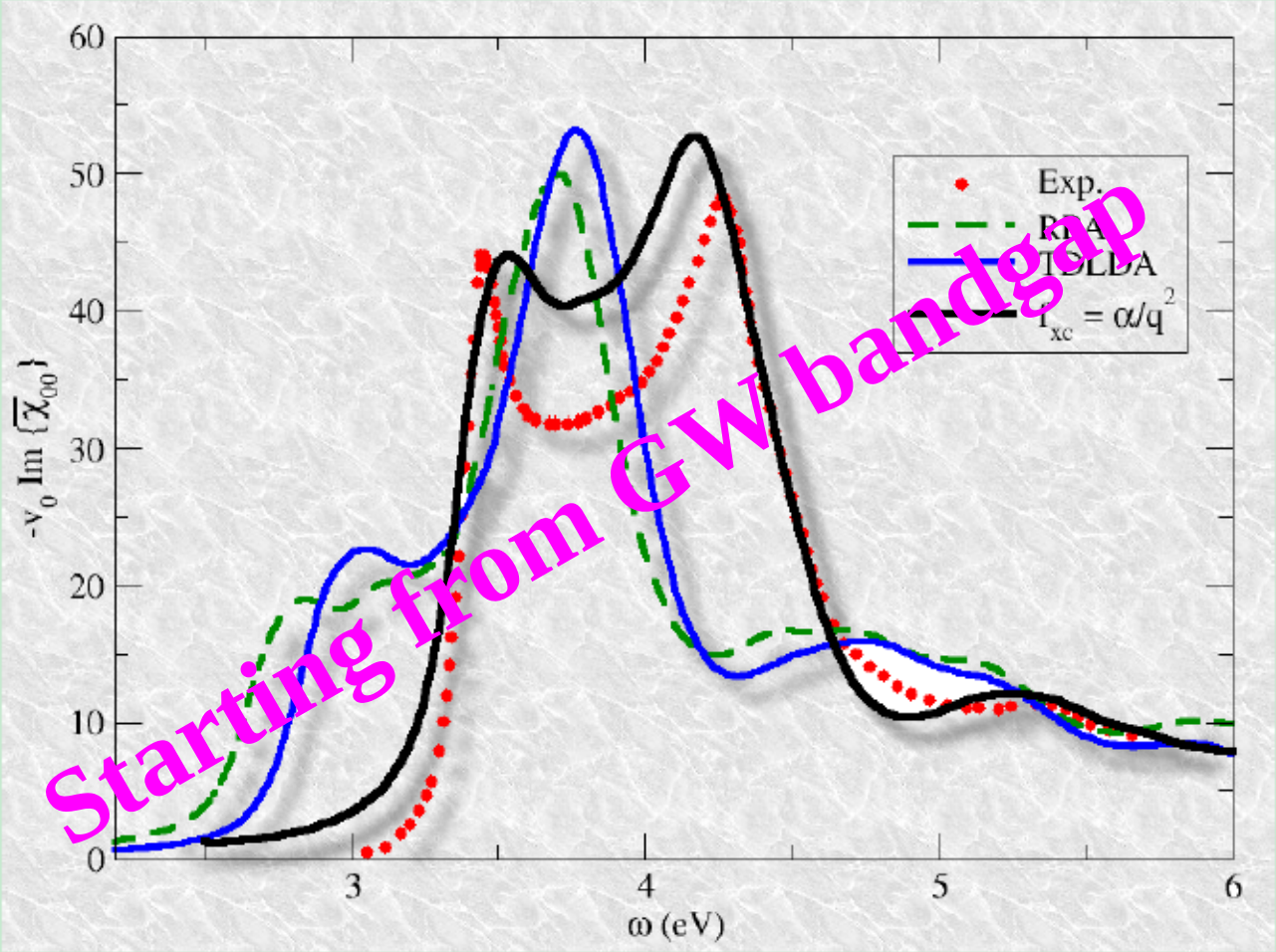
Absorption of Silicon $f_{xc} = \frac{\alpha}{q^2}$



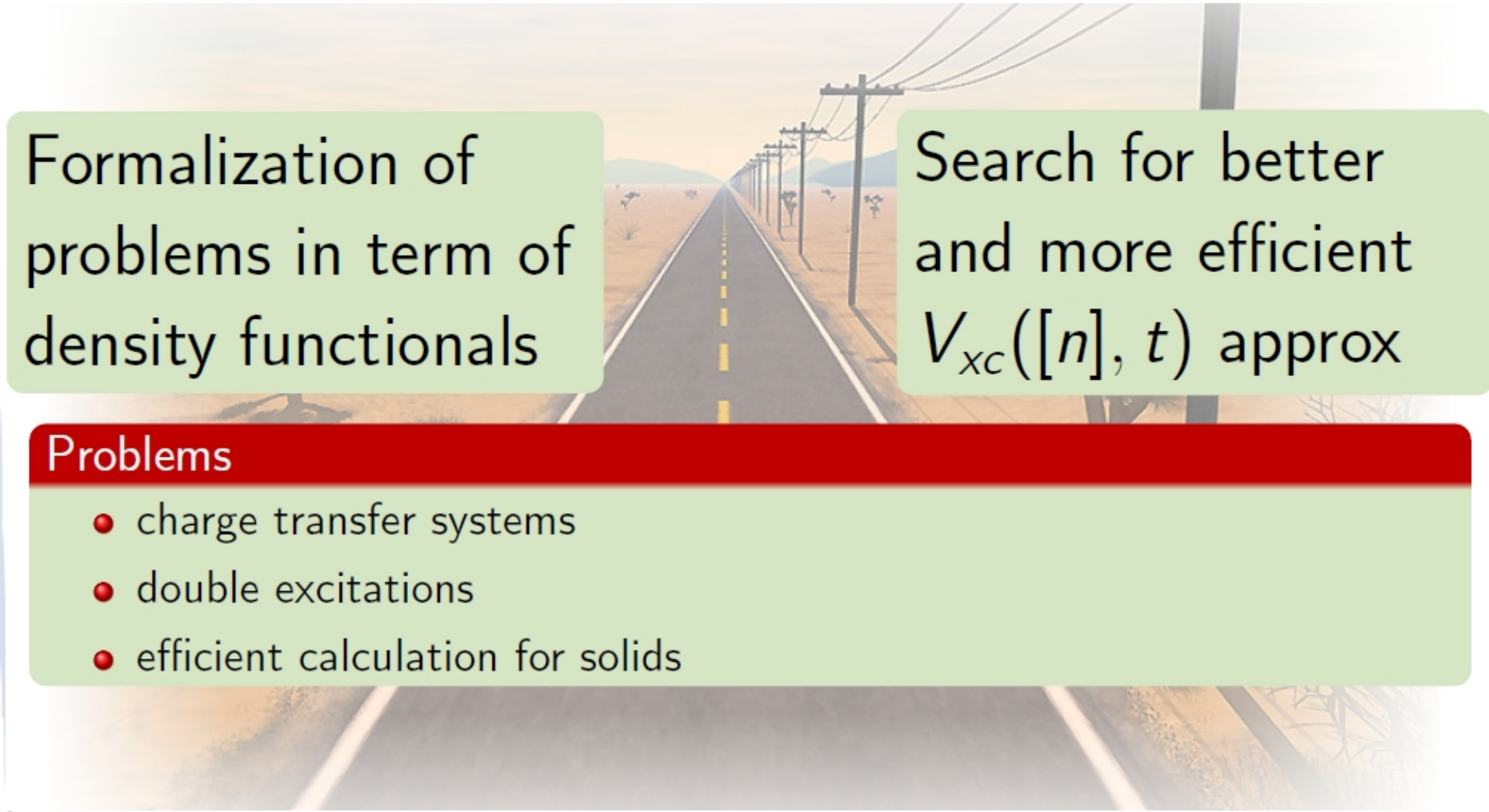
L.Reining *et al.* Phys.Rev.Lett. **88**, 66404 (2002)

ALDA: Achievements and Shortcomings

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



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



Formalization of problems in term of density functionals

Search for better and more efficient $V_{xc}([n], t)$ approx

Problems

- charge transfer systems
- double excitations
- efficient calculation for solids

Also:

* total energies

* transport

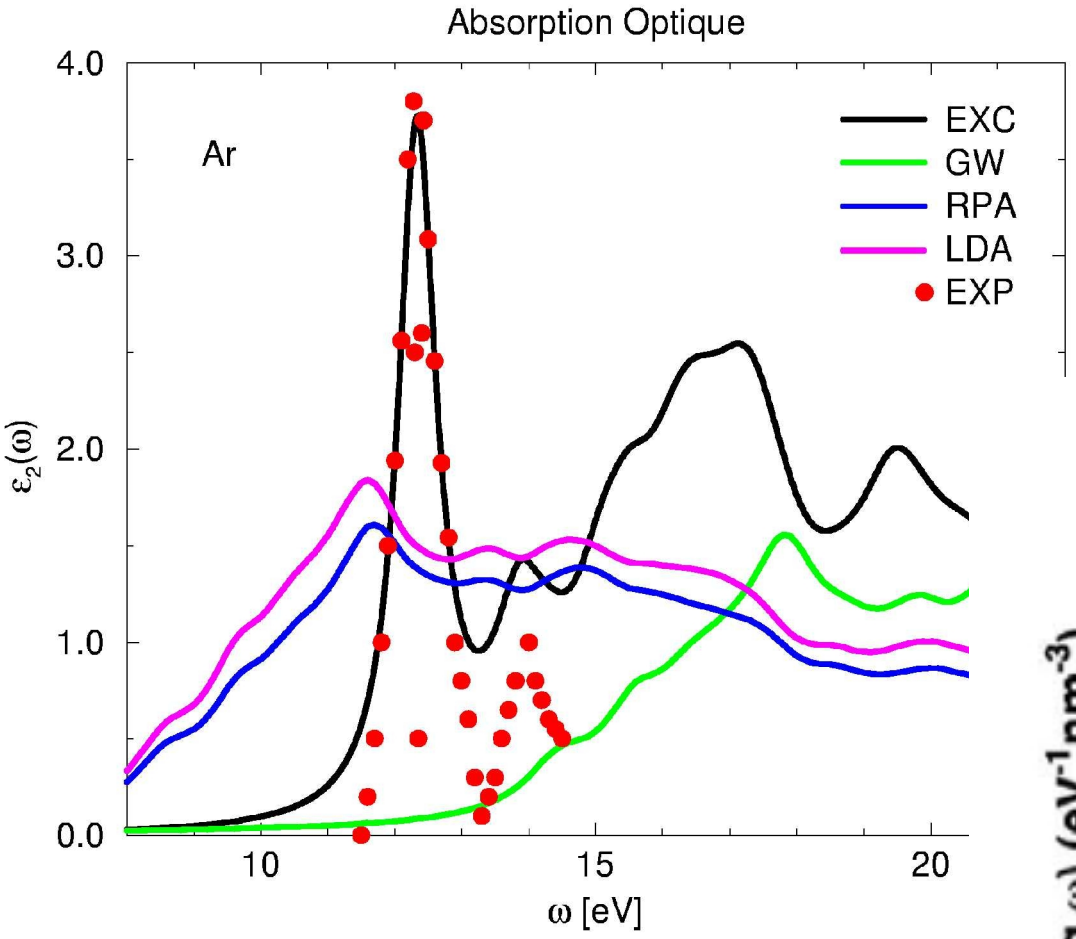
* feed in MBPT

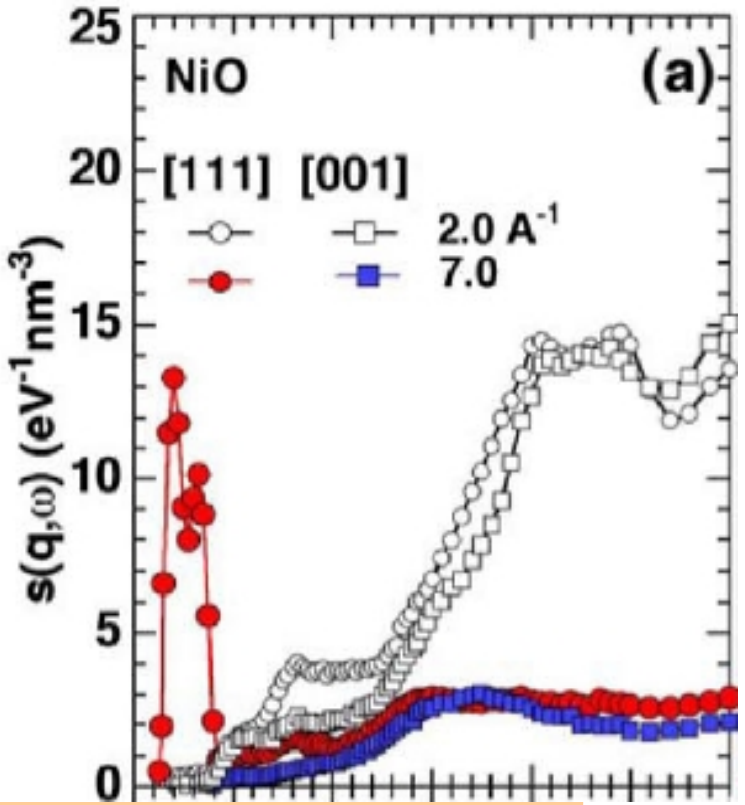
*.....

Notes:

* Finite systems and correlation

* The “bandgap problem”



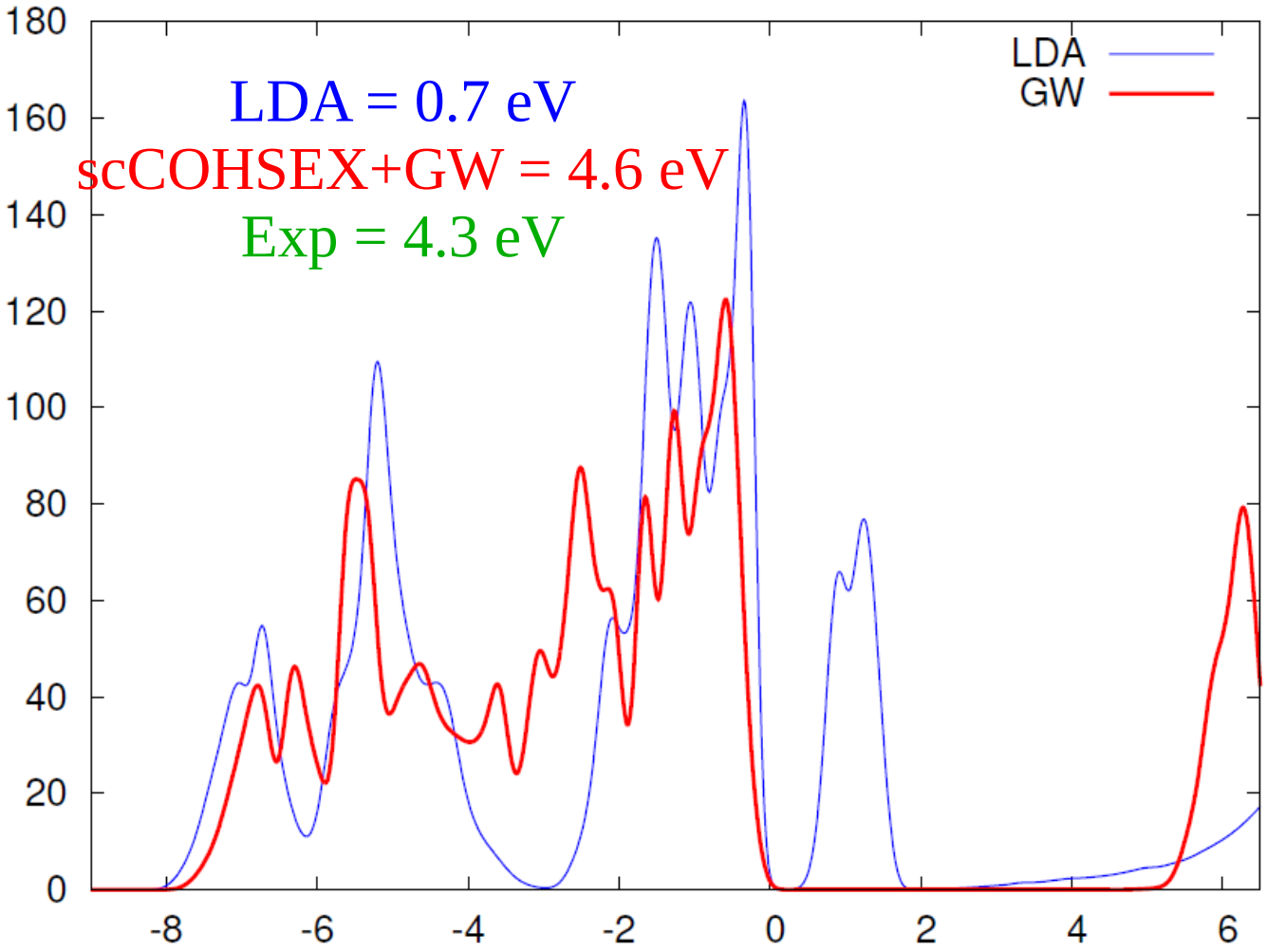


V. Olevano et al. (2000)
(bulk silicon 1998)

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

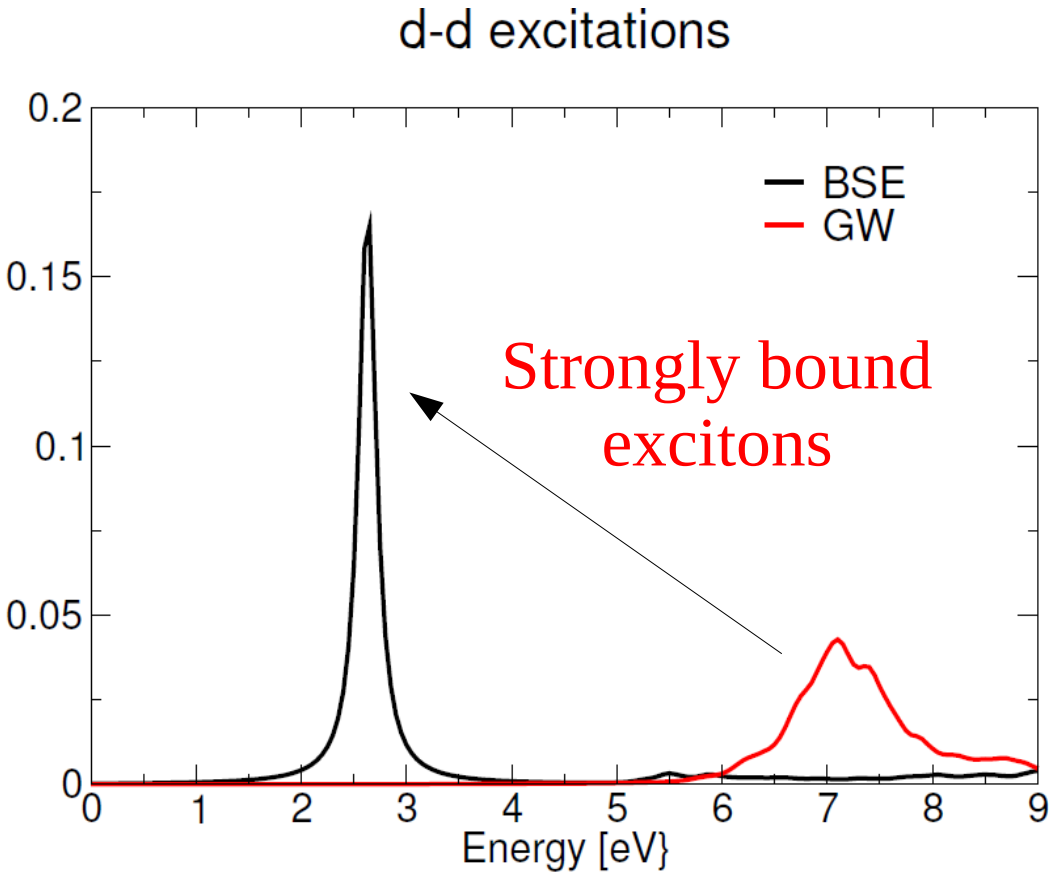
Exciton: Lee, Hsueh, Ku, PRB 82, 081106 (2010)

NiO: density of states



M. Guzzo, Master thesis (2008)

NiO: dd excitations

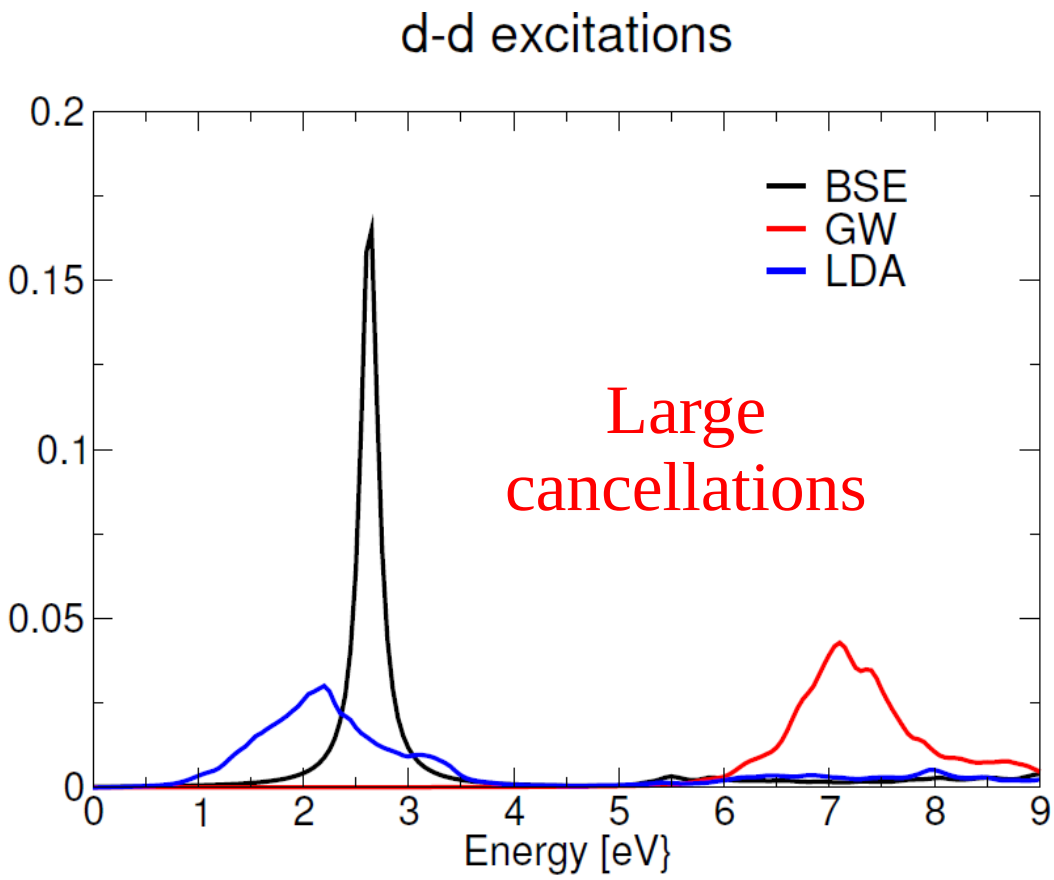


Q ~ 8 Å^{-1} [111]

M. Gatti et al. (2014)

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

NiO: dd excitations

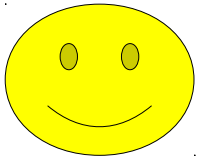


Notes:

* Finite systems and correlation

* The “bandgap problem”

* Excitons are fake!



Notes:

* Finite systems and correlation

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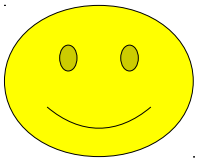

* double excitations → dynamical effects

$$f_{xc}(r,r',t-t') \rightarrow f_{xc}(r,r',\omega)$$

Codes (more or less) available for TDDFT

- DP (Olevano,Reining,Sottile) - (reciprocal space, frequency domain) - solides and finite systems - Academic Free License
  http://etsf.polytechnique.fr/Software/Ab_Initio
- Octopus (Marques,Castro,Rubio) -(real space, real time) - finite systems
- Yambo (Marini Grüning Attaccalite Varsano Hogan) - (reciprocal space, frequency domain)
- Fiesta (Blase) - (Gaussian based, frequency domain) - finite systems
- Fleszar code
- Rehr (core excitations)
- TDDFT (Bertsch)
- VASP, SIESTA, ADF, TURBOMOLE
- TD-DFPT (Baroni)

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- TD-DFPT (Baroni)

EXCITING!!!!!

Time Dependent Density Functional Theory

→ Why bother?	*It all depends on the response*
→ Intuitive	*could do without theory....*
→ More formally	*to go further*
→ Approximations	*always the same*
→ Realizations	*choose your space*
→ Applications	*broad range*
→ Notes	*remember your basics!*

http://etsf.polytechnique.fr