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ICTP 40th Anniversary

SMR 1564 - 5

SPRING COLLEGE ON SCIENCE AT THE NANOSCALE
(24 May - 11 June 2004)

TDDFT THEORY:

APPLICATIONS TO NANO AND BIO-STRUCTURES

Optical Properties of Nanostructures: Extended systems: problems and new developments

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Optical properties of nanostrutures

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I. Motivation. Basic concepts. Foundations TDDFT.

II. Illustration of the physics for nano- and bio structures

III. Extended systems: problems and new developments

ICTP Spring College on Science at the Nanoscale, Trieste May 24th -June 11th 2004

Optical properties of nanostrutures

III. Extended systems: problems and new developments

Introduction:

how to handle the electron dynamics in extended systems under the influence of an external electromagnetic field?

TDDFT:

- *Problems with standard exchange-correlation functionals*
- *A new fxc derived from Many-body perturbation theory*
  proper description of excitonic effecs!!!
- *Applications to poliacetilene as one-dimensional system*

G. Onida, L. Reining and AR, Rev. Mod. Phys. ***74****, 601 (2002)*

Time-dependent approach for extended systems: a gauge formalism

G.F. Bertsch, J.I. Iwata, AR, K. Yabana, PRB62, 7998 (2000)

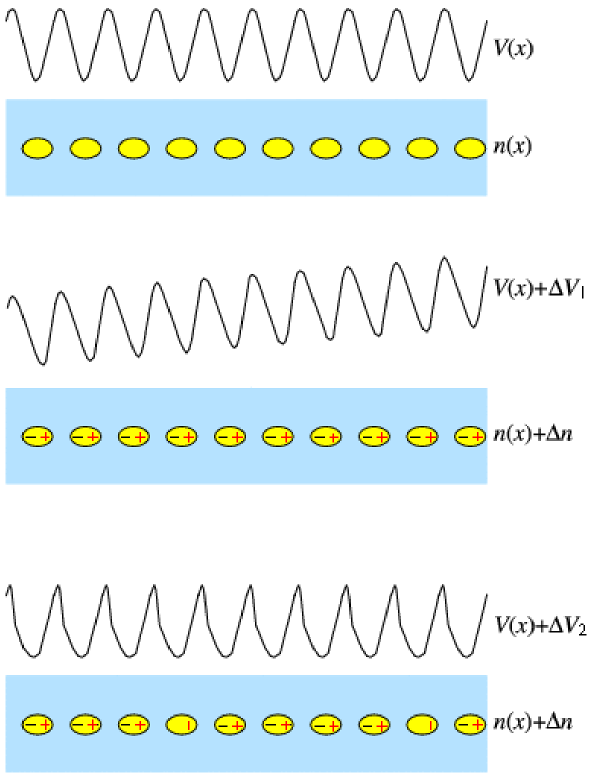
The Lagrangian of a periodic system in a volume V under a uniform field is

$$L=\sum_i <\psi_i|i\hbar\frac{\partial}{\partial t}-\frac{1}{2m}(\vec{p}+\frac{e}{c}\vec{A})^2-V_{ion}|\psi_i>-E_{Hartree}-E_{xc}+\frac{V}{8\pi c^2}(\frac{d\vec{A}}{dt})^2$$

The equation of motion are:

$$i\hbar\frac{\partial}{\partial t}\psi_i=\left[\frac{1}{2m}(\vec{p}+\frac{e}{c}\vec{A})^2+V_{ion}+V_H+V_{xc}\right]\psi_i$$

$$\frac{d^2\vec{A}}{dt^2}=-4\pi e^2\frac{n}{m}\vec{A}-4\pi c\frac{e}{V}\sum_i <\psi_i|\frac{\vec{p}}{m}|\psi_i>$$



For the electric field is:

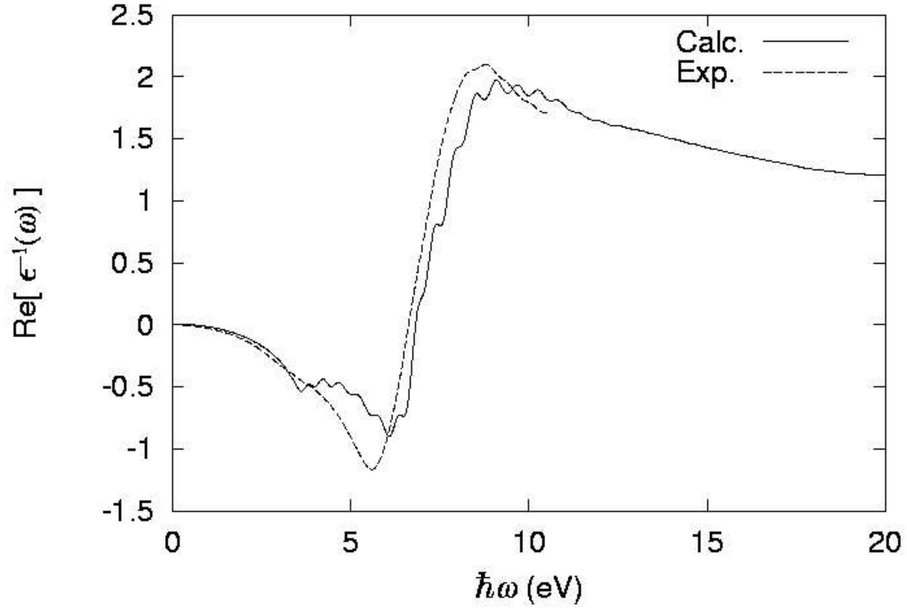
$$\vec{E}(t)=\frac{-1}{c}\frac{d\vec{A}}{dt}$$

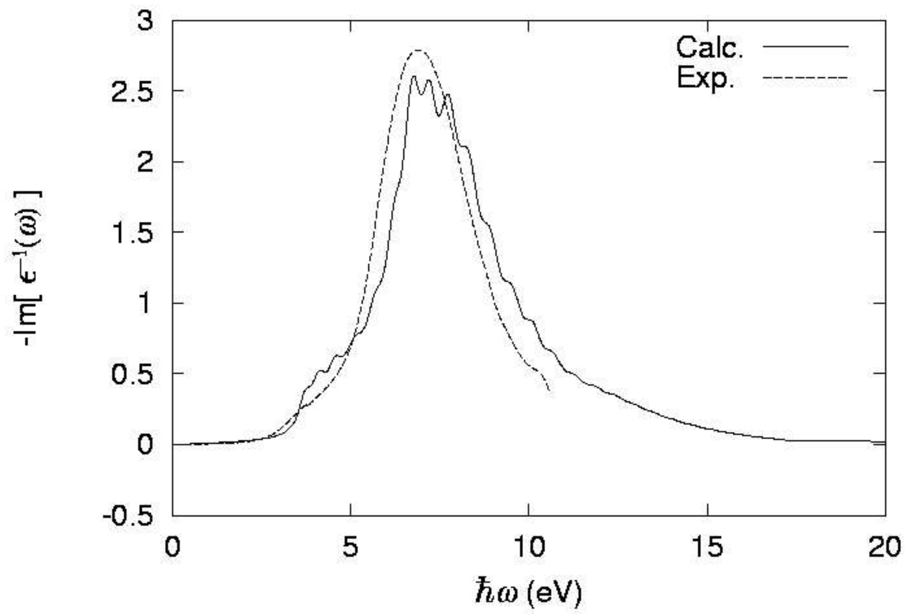
$$\frac{d\vec{E}}{dt}=-4\pi\vec{j}$$

and

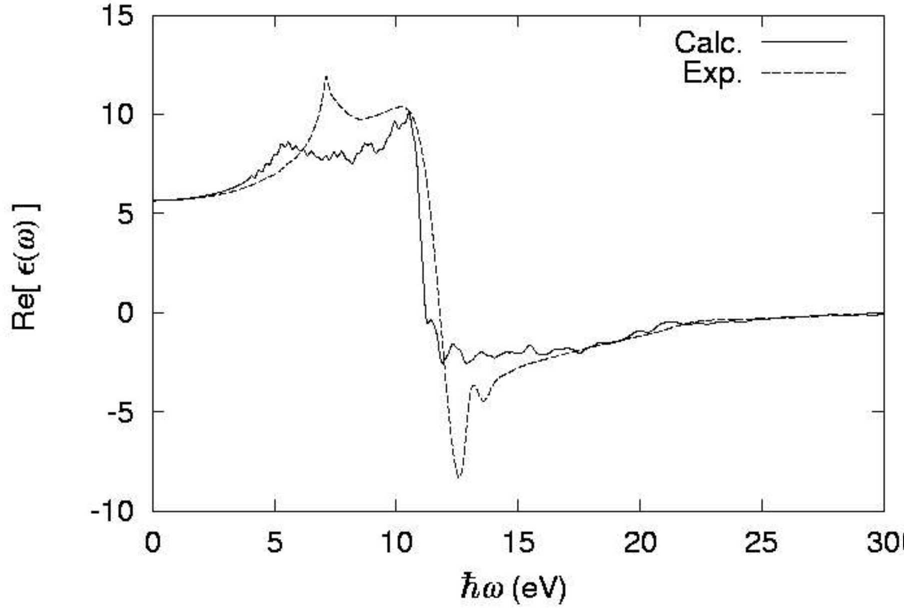
$$\vec{j}=\frac{-e}{V}\sum_i <\psi_i|\frac{\vec{p}}{m}|\psi_i>-\frac{e^2}{c}n\vec{A}$$

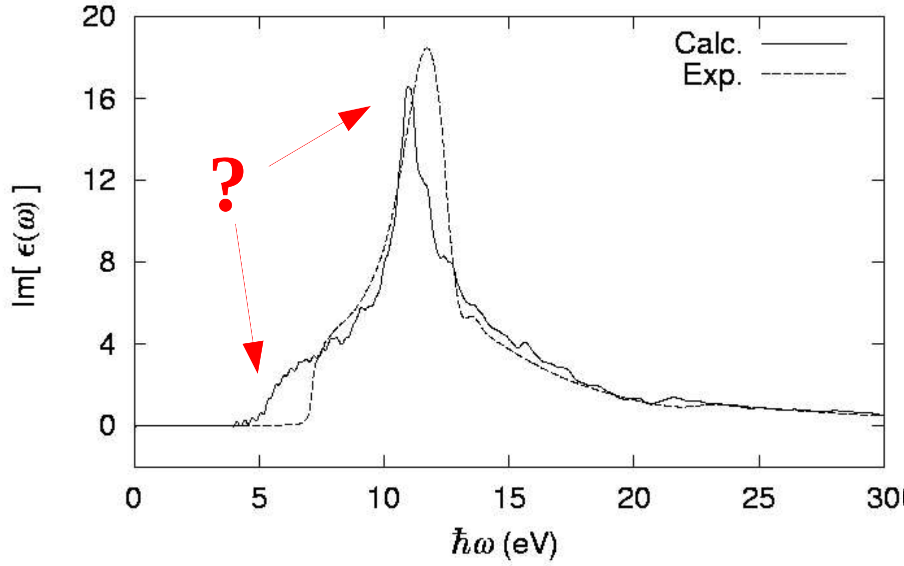
Lithium





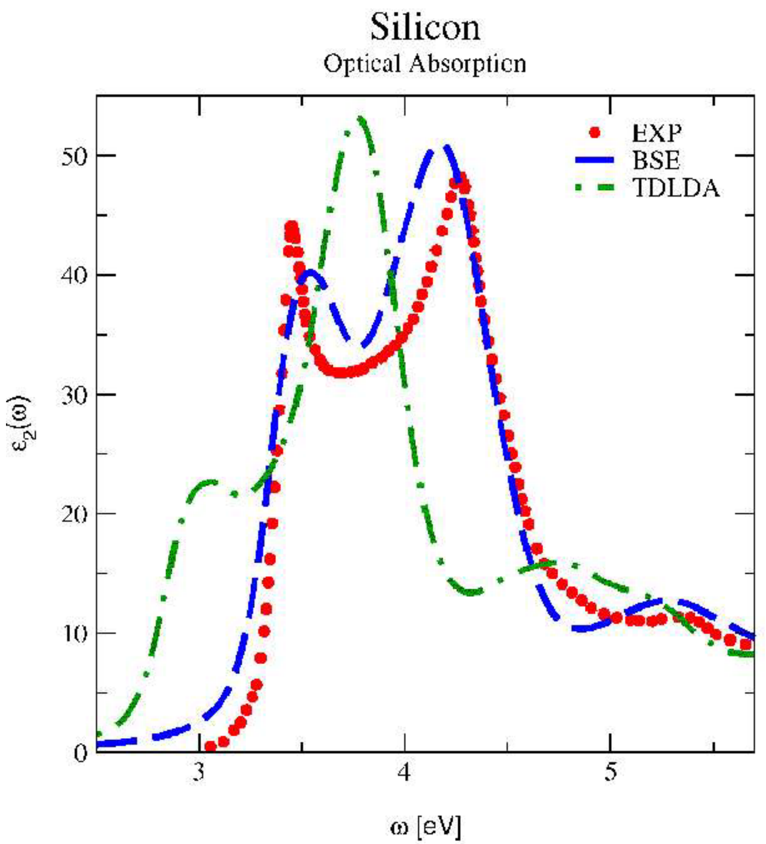
Diamond





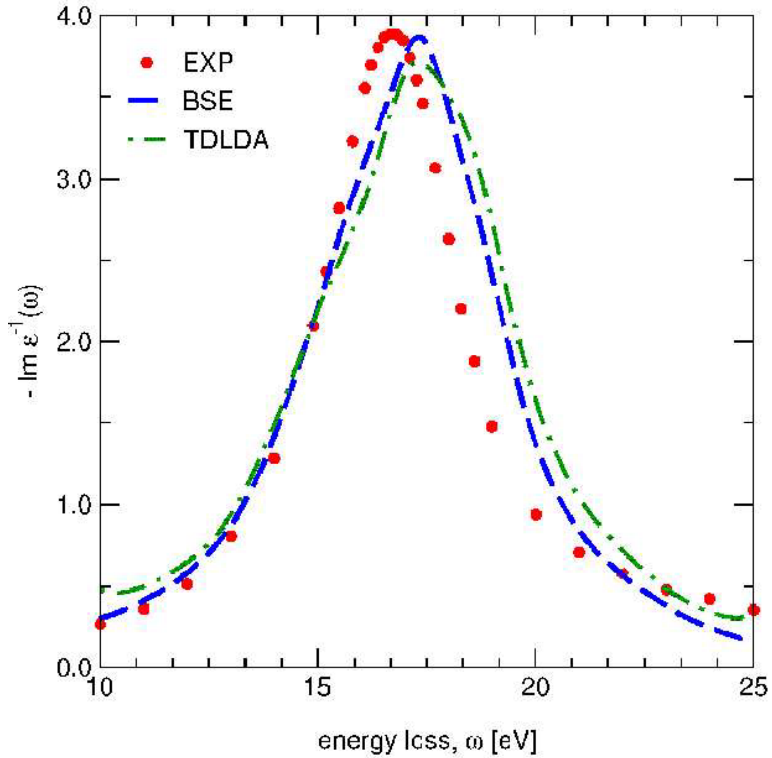
Non-local fxc for extended systems:

Motivation



The LDA Kernel is not able to reproduce Optical Properties in Solids

BSE vs TDLDA comparison on EEL



The LDA Kernel already offers a good representation of the Electron Energy Loss (EEL) spectrum in Solids

See for a review: G. Onida, L. Reining and AR, Rev. Mod. Phys. ***74****, 601 (2002)*

Why a non-local (static?) fxc for extended systems:

$$f_{xc} = -\alpha(\omega)/q^2$$

- In the EEL spectra f_{xc} is added to the full coulomb that already contains a long range contribution

$$EEL \, \alpha \, \epsilon^{-1}(\omega) = 1 + v\chi$$

$$\chi(\omega) = \chi_0(\omega) + \chi_0(\omega)(v + f_{xc}(\omega))\chi(\omega)$$

- In the absorption spectra f_{xc} is added to the full coulomb that does not contains the long range contribution (q=0)

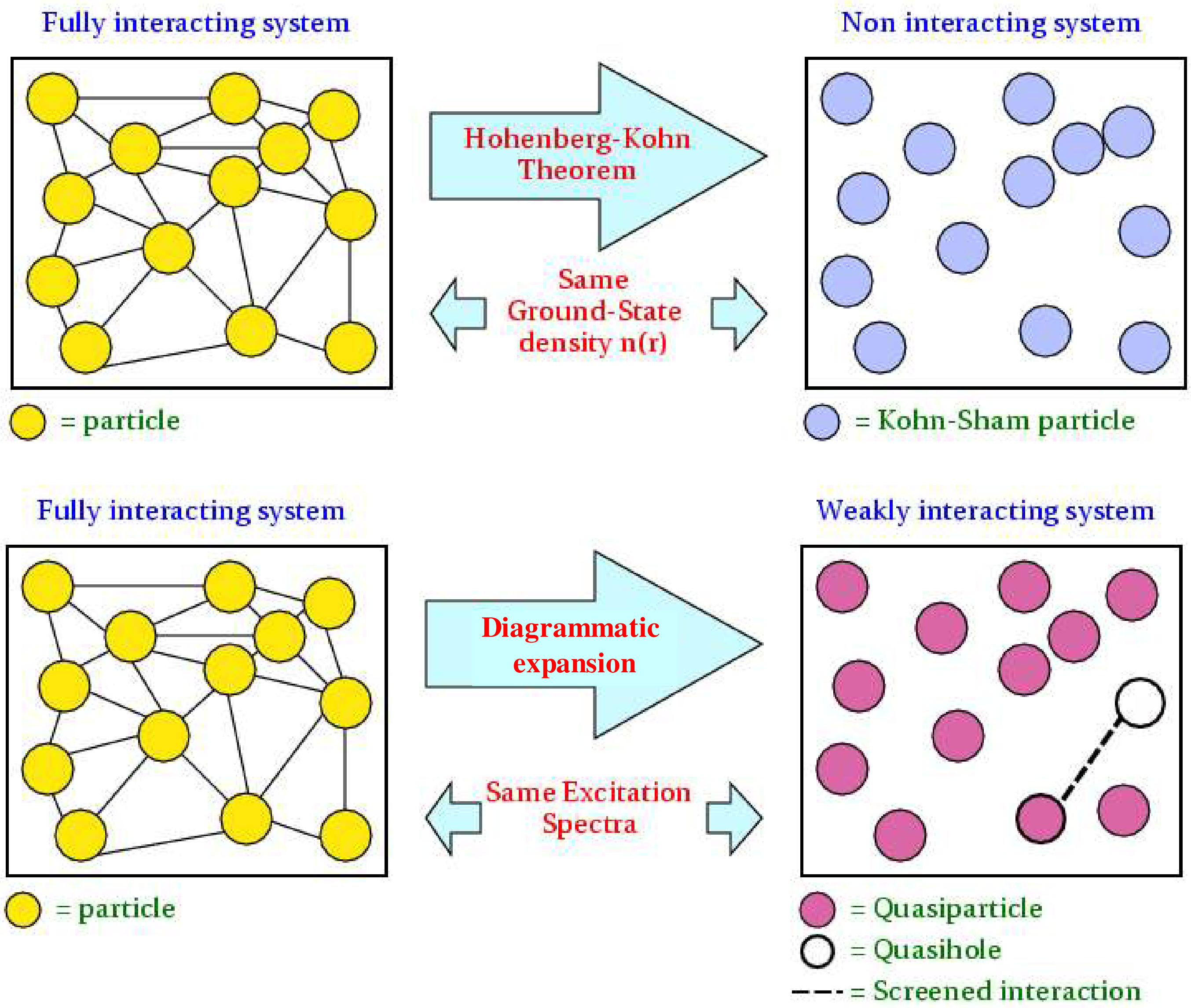
$$\epsilon_M(\omega) = 1 - v\bar{\chi} \qquad \epsilon_M^{RPA} \equiv 1/[1 - v\chi_0]_{G=G'=0}$$

$$\bar{\chi}(\omega) = \chi_0^{GW}(\omega) + \chi_0^{GW}(\omega)(\bar{v} + f_{xc}(\omega))\bar{\chi}(\omega)$$

*The **lack** of a **long range term** in f_{xc}^{LDA} is relatively weightless in the EEL but is crucial in the absorption spectra!!!*

*L. Reining, V. Olevano, AR, G. Onida, PRL**88**, 0664041 (2002); S. Botti et al, PRB (2004).*

Density Functional versus Many-body perturbation theory



Band-gap problem!!!!!

Density Functional Theory and Many-Body Perturbation Theory

$$\left[-\frac{\nabla^2}{2}+V_{ext}(\mathbf{r})+V_{Hartree}([n],\mathbf{r})+V_{xc}([n],\mathbf{r})\right]\phi_i(\mathbf{r})=\epsilon_i\phi_i(\mathbf{r})$$

R. O. Jones and O. Gunnarsson, Rev. Mod. Phys. **61**, 689 (1989)

$$V_{xc}([n],\mathbf{r})=\frac{\delta E_{xc}[n]}{\delta n(\mathbf{r})} \qquad E_{xc}^{LDA}[n]=\int d\mathbf{r}\, n(\mathbf{r})\,\epsilon_{xc}^{hom}([n];\mathbf{r})$$

Density Functional Theory

Exchange-correlation Potential: Real, Local in space, Frequency independent

Self-Energy: Complex, Non-local in space, Frequency dependent

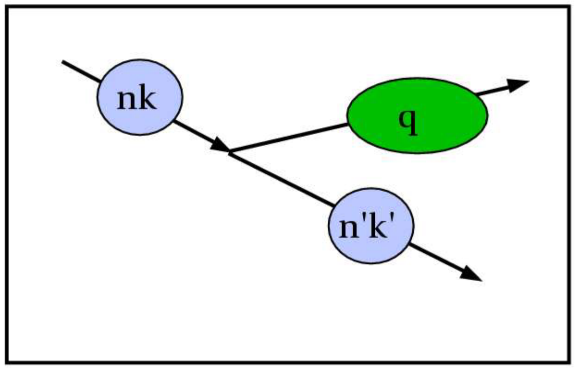
Many-Body Perturbation Theory

$$[\mathcal{H}_{KS}-V_{xc}(\mathbf{r})](\mathbf{r})\,\phi_i(\mathbf{r};E_\lambda)+\int d\mathbf{r}'\Sigma(\mathbf{r},\mathbf{r}';E_\lambda)\,\phi_i(\mathbf{r}';E_\lambda)=E_\lambda(\omega)\,\phi_\lambda(\mathbf{r},E_\lambda)$$

*G. Onida, L. Reining and AR, Rev. Mod. Phys. **74**, 601 (2002)*

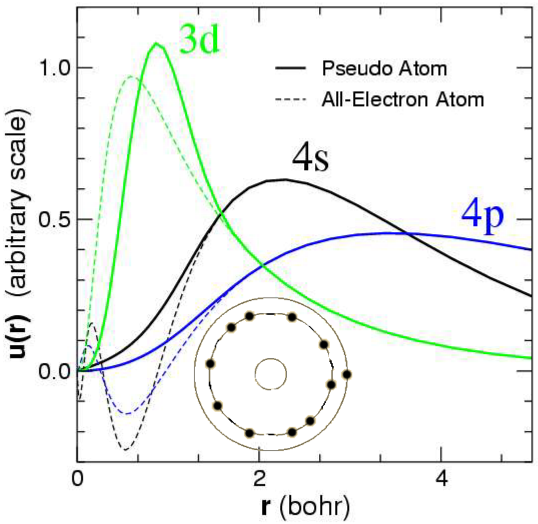
F. Aryasetiawan, Rep. Prog. Phys. **61**, 237-312 (1998)

The self-energy physics

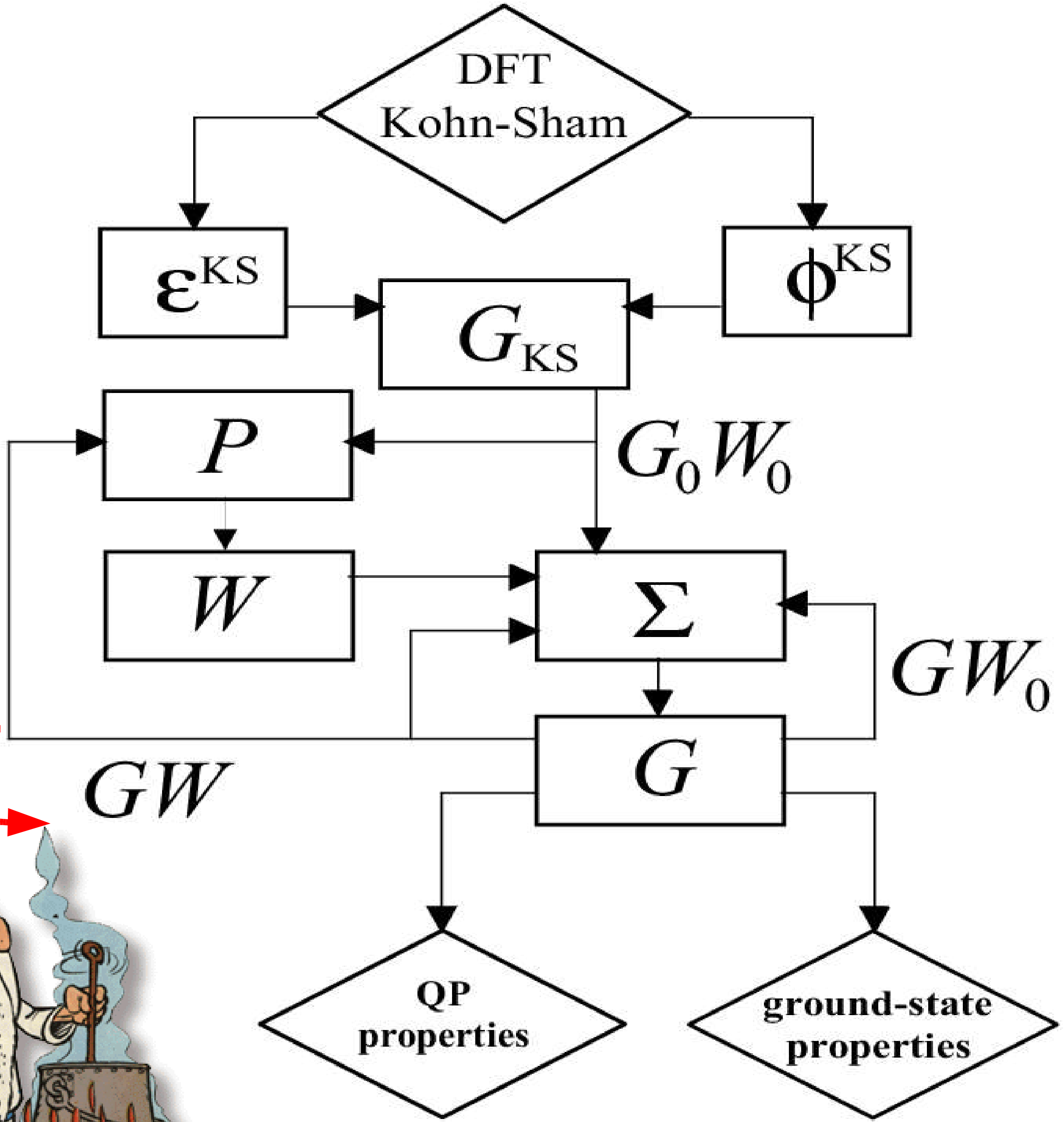


=Kohn-Sham states
=Plasmons/Electron-hole states

The pseudopotential approach



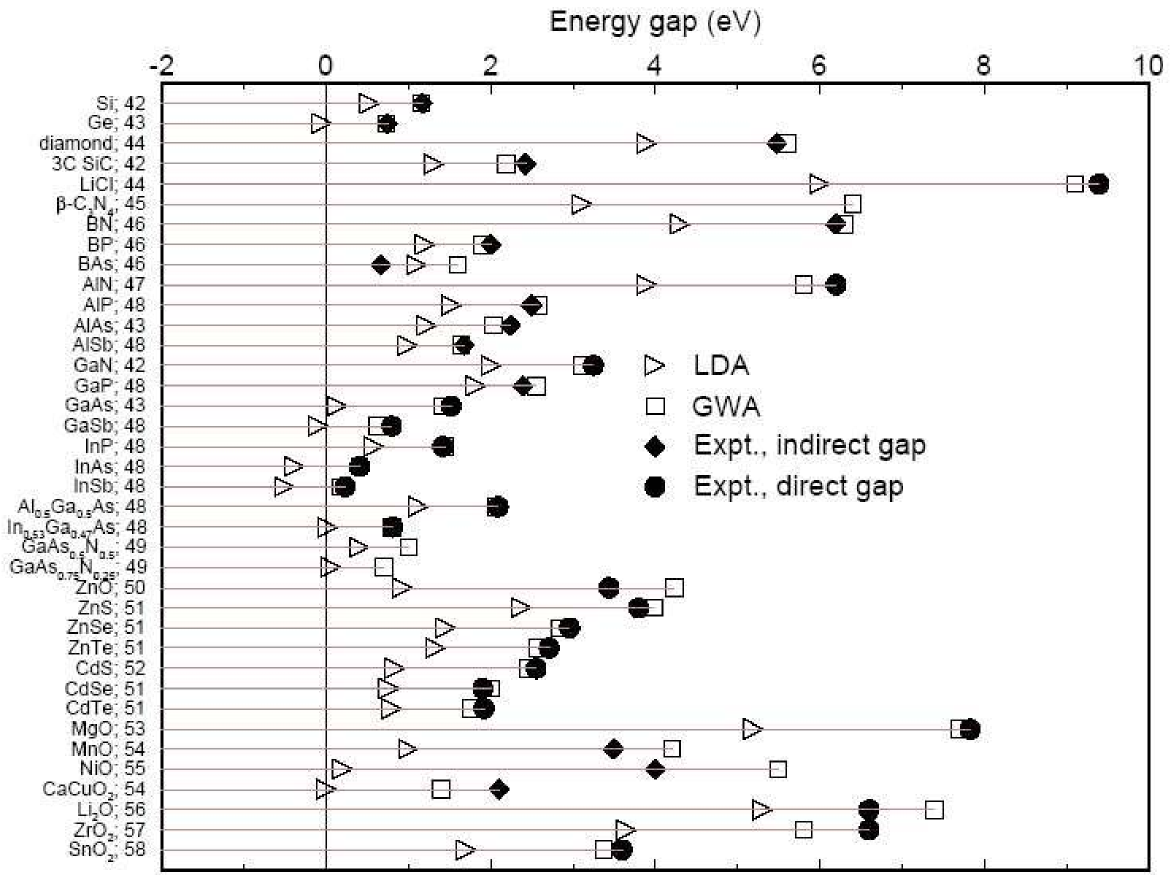
The GW "soup"



$$P(1\,2) = -iG(1\,2)\,G(2\,1^+)$$

$$\Sigma(1\,2) = iG(1\,2^+)\,W(1\,2)$$

G_0W_0 Band Structures of Insulators



$$E_n^{QP} \simeq \epsilon_n^{KS} + < \psi_n \left| \Sigma(\epsilon_n^{KS}) - V_{xc} \right| \psi_n >$$

From "Quasiparticle calculations in solids", W.G. Aulbur, L. Jönsson and J.W. Wilkins, Solid State Physics 54 1 (2000),

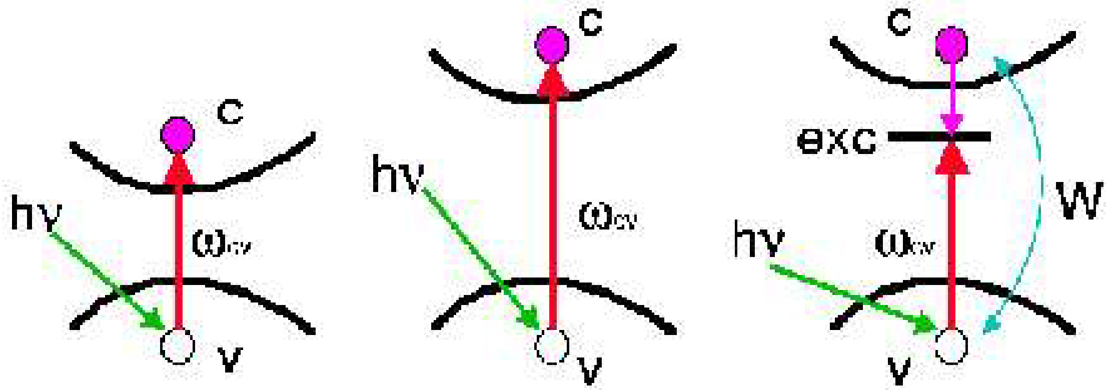
also available in preprint form at http://www.physics.ohio-state.edu/~wilkins/vita/publications.html#reviews

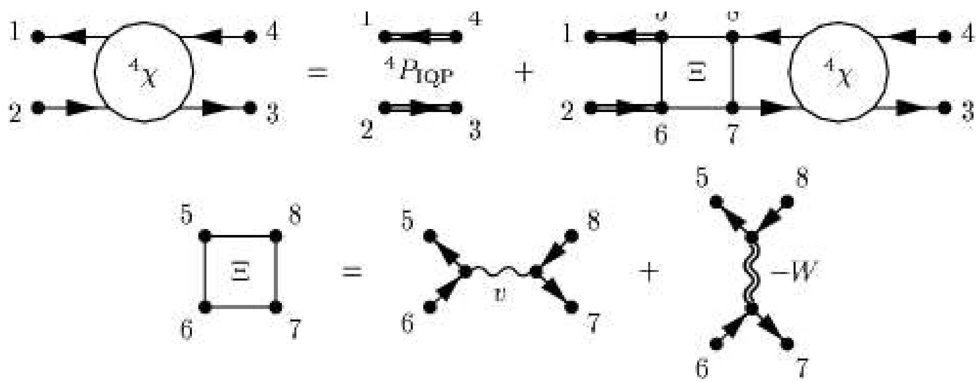
Bethe-Salpeter equation: excitonic effects

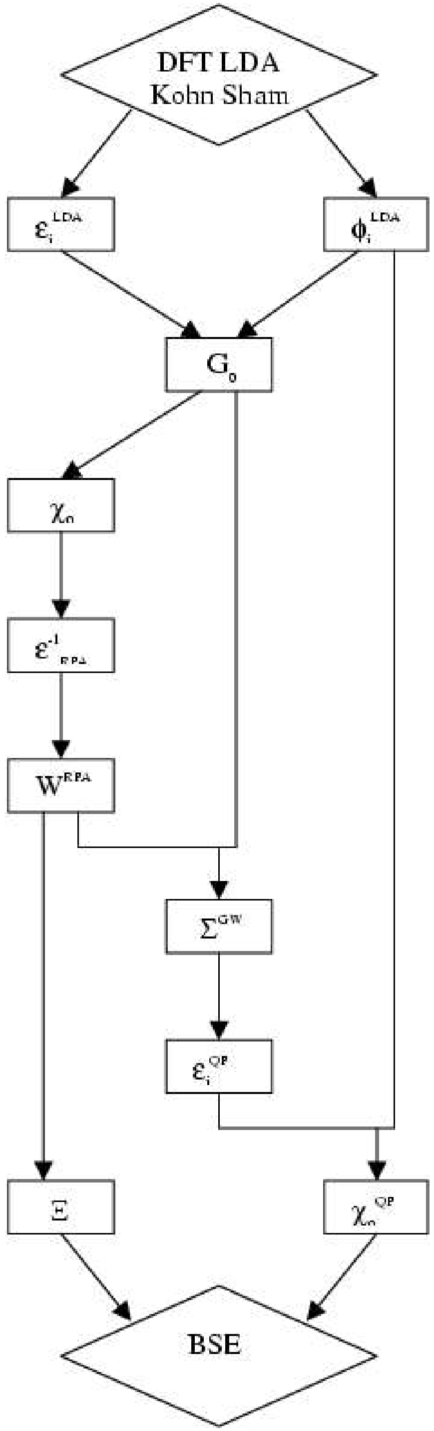
$$\Sigma = iG_0W_0 ; W_0 = \epsilon_{RPA}^{-1} v$$

$$\epsilon_{RPA} = 1 - v_c \chi^{(0)}$$

$$\chi^{(0)}(r, r', \omega) = 2\, \Sigma_{i \neq j} (f_i - f_j) \frac{\varphi_i(r)\varphi_j(r)\phi_i^*(r')\phi_j(r')}{\epsilon_i - \epsilon_j - \omega - i\eta}$$

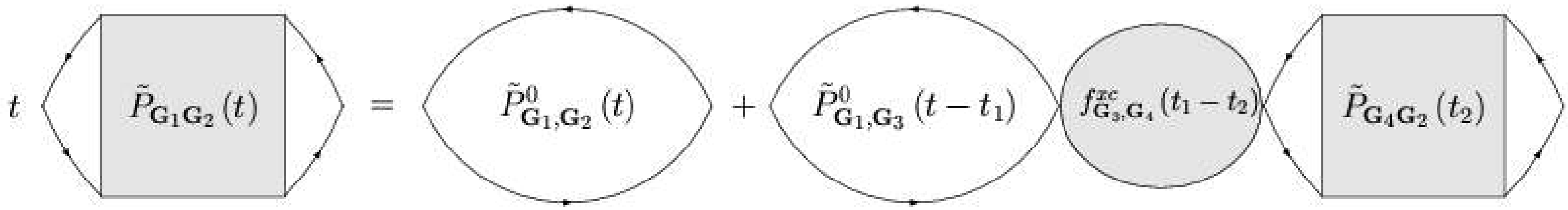




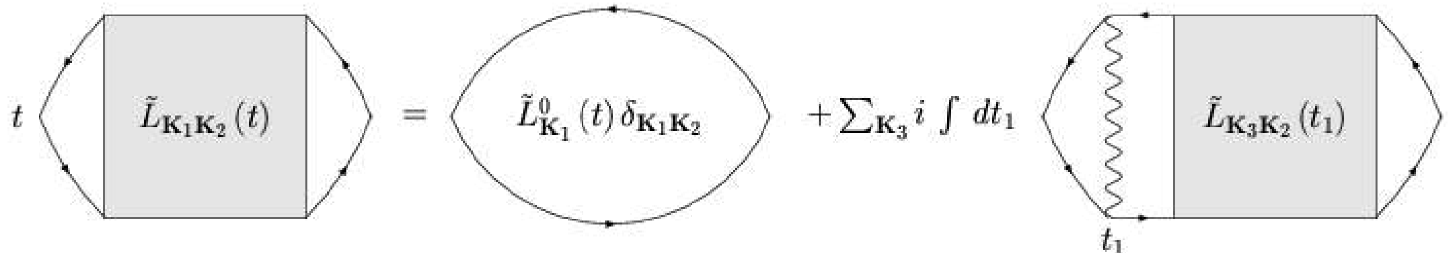


*G. Onida, L. Reining and AR, Rev. Mod. Phys. **74**, 601 (2002)*

TDDFT ...



$$\iint d\mathbf{r}_2\, d\mathbf{r}_3 \chi_s(\mathbf{r}_1,\mathbf{r}_2;\omega)\left[\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}+f^{xc}(\mathbf{r}_2,\mathbf{r}_3;\omega)\right]\xi(\mathbf{r}_3;\omega)=\lambda(\omega)\,\xi(\mathbf{r}_1;\omega) \qquad \lambda(E_\lambda)=1$$



$$\mathbf{K}_1 \equiv \{c_1, v_1, \mathbf{k}_1\}$$

$$\tilde{P}_{\mathbf{G}_1,\mathbf{G}_2}(\omega) \propto \sum_{\mathbf{K}_1,\mathbf{K}_2} \Phi^*_{\mathbf{K}_1}(\mathbf{G}_1)\, L_{\mathbf{K}_1,\mathbf{K}_2}(\omega)\, \Phi_{\mathbf{K}_2}(\mathbf{G}_2) \qquad \Phi_{\mathbf{K}_1}(\mathbf{G}_1)=\langle c_1\mathbf{k}_1|e^{\mathbf{G}_1\cdot\mathbf{r}}|v_1\mathbf{k}_1\rangle$$

$$\tilde{P}_{\mathbf{G}_1,\mathbf{G}_2}(\omega) \propto \sum_\lambda \frac{\Phi^*_\lambda(\mathbf{G}_1)\,\Phi_\lambda(\mathbf{G}_2)}{\omega - E_\lambda} \qquad \mathbf{H}|\lambda\rangle = E_\lambda|\lambda\rangle \qquad H_{\mathbf{K}_1,\mathbf{K}_2} = (\epsilon_{c_1\mathbf{k}_1}-\epsilon_{v_1\mathbf{k}_1})\,\delta_{\mathbf{K}_1,\mathbf{K}_2} + iW_{\mathbf{K}_1,\mathbf{K}_2}$$

... and Many-Body Perturbation Theory

Many-Body approach to the Exchange-Correlation Kernel of TDDFT

A diagrammatic approach

Hypothesis

It exists a "many-body xc-kernel" such that
the TDDFT and Many-Body polarization
functions are identical

Consequently TDDFT equation can be used as an equation for the xc-kernel and as a formal solution can be found in terms of an iterative equation for the nth order contribution

A. Marini, R. Del Sole and AR, PRL (2003)

Many-Body approach to the Exchange-Correlation Kernel of TDDFT

TDDFT

$$\tilde{\mathbf{P}}(\mathbf{q},\omega) = \mathbf{P}^{(0)}(\mathbf{q},\omega) + \mathbf{P}^{(0)}(\mathbf{q},\omega)\,\mathbf{f}_{xc}(\mathbf{q},\omega)\,\tilde{\mathbf{P}}(\mathbf{q},\omega)$$

$$\tilde{P}_{\mathbf{G}_1,\mathbf{G}_2}(\mathbf{q},\omega) = const.\sum_{\mathbf{K}_1,\mathbf{K}_2} \Phi^*_{\mathbf{K}_1}(\mathbf{q},\mathbf{G}_1)\,\tilde{S}_{\mathbf{K}_1,\mathbf{K}_2}(\mathbf{q},\omega)\,\Phi_{\mathbf{K}_2}(\mathbf{q},\mathbf{G}_2)$$

MBPT

$$\tilde{\mathbf{S}}(\mathbf{q},\omega) = \mathbf{S}^{(0)}(\mathbf{q},\omega) + \mathbf{S}^{(0)}(\mathbf{q},\omega)\,\mathbf{W}(\mathbf{q})\,\tilde{\mathbf{S}}(\mathbf{q},\omega)$$

$$\Phi_{\mathbf{K}}(\mathbf{q},\mathbf{G}) = \langle c\mathbf{k}|e^{i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}}|v\mathbf{k}-\mathbf{q}\rangle \qquad \mathbf{K} := (c\,v\,\mathbf{k})$$

Bethe-Salpeter Equation

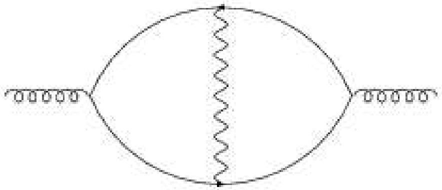
$$\mathbf{f}^{(n)}_{xc}(\mathbf{q},\omega) = \frac{1}{\mathbf{P}^{(0)}(\mathbf{q},\omega)}\left[\delta\tilde{\mathbf{P}}^{(n)}(\mathbf{q},\omega)\left(\mathbf{P}^{(0)}(\mathbf{q},\omega)\right)^{-1} - \sum_{m=1,n-1}(-1)^m\,\delta\tilde{\mathbf{P}}^{(m)}(\mathbf{q},\omega)\,\mathbf{f}^{(n-m)}_{xc}(\mathbf{q},\omega)\right]$$

Iterative equation for f_{xc}

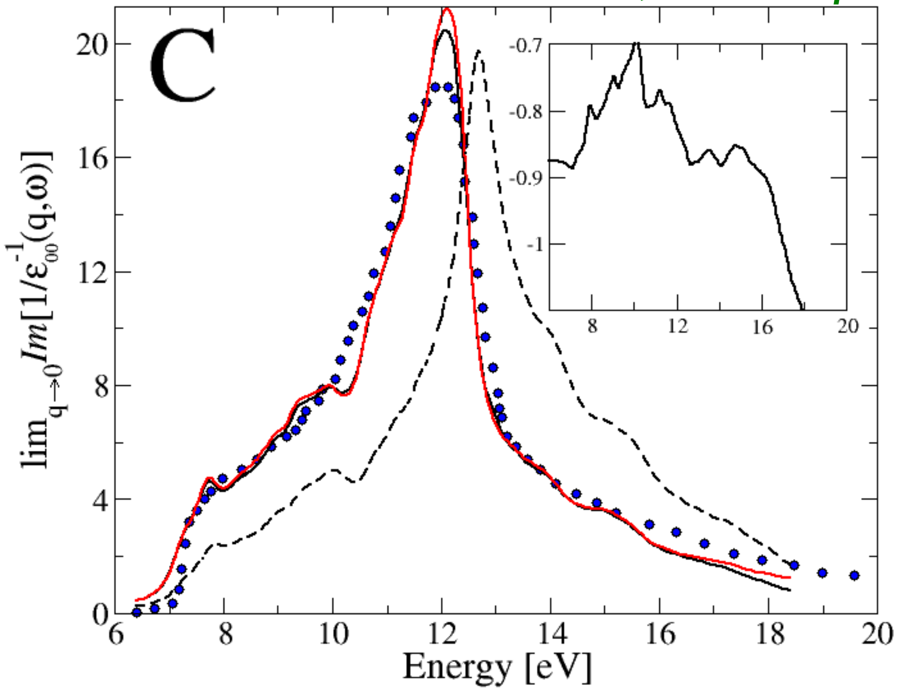
$$\mathbf{f}_{xc}(\mathbf{q},\omega) = \sum_n \mathbf{f}^{(n)}_{xc}(\mathbf{q},\omega) \qquad \mathbf{f}^{(0)}_{xc}(\mathbf{q},\omega) = 0$$

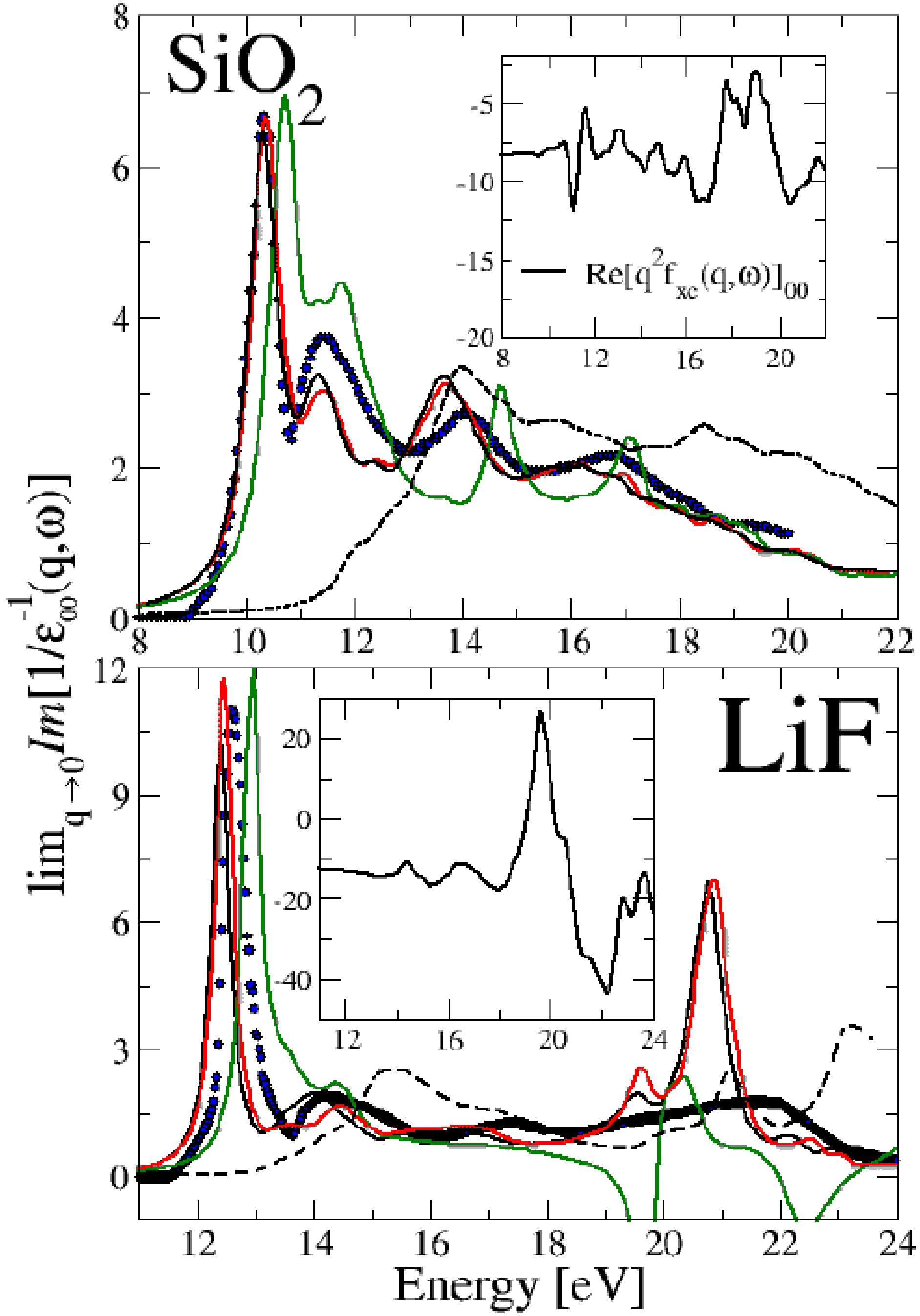
A. Marini, R. Del Sole and AR, PRL (2003)

Bound excitons in TDDFT

$\mathbf{f}_{xc}^{(1)}(\mathbf{q},\omega) =$ 

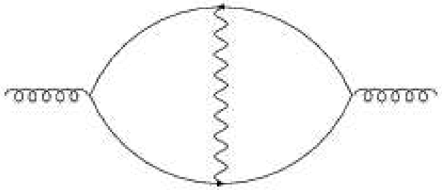
 $:= \left[\mathbf{P}^{(0)}(\omega)\right]^{-1}$

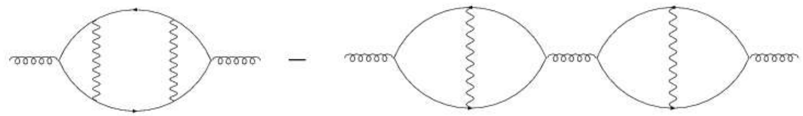


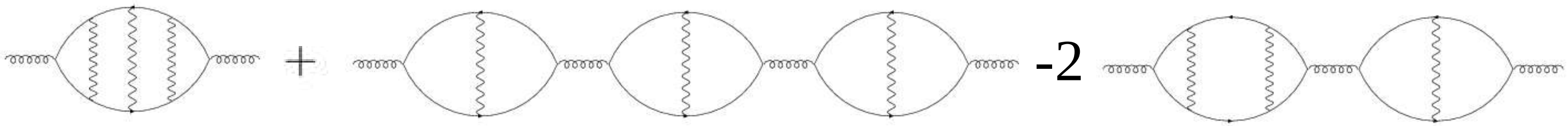


A. Marini, R. Del Sole and AR, PRL (2003)

How many terms ?

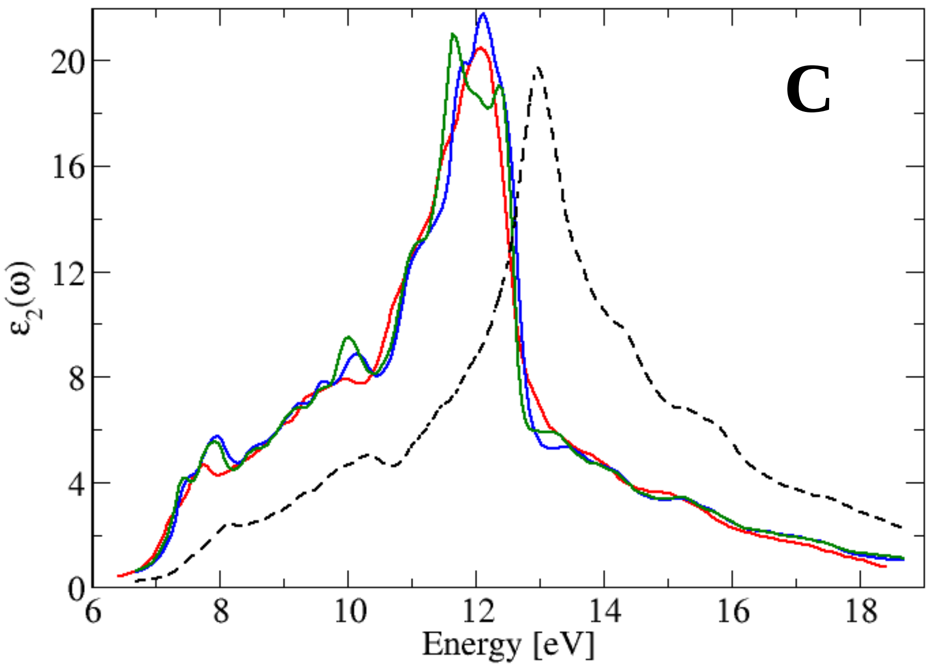
$\mathbf{f}_{xc}^{(1)}(\mathbf{q},\omega) =$ 

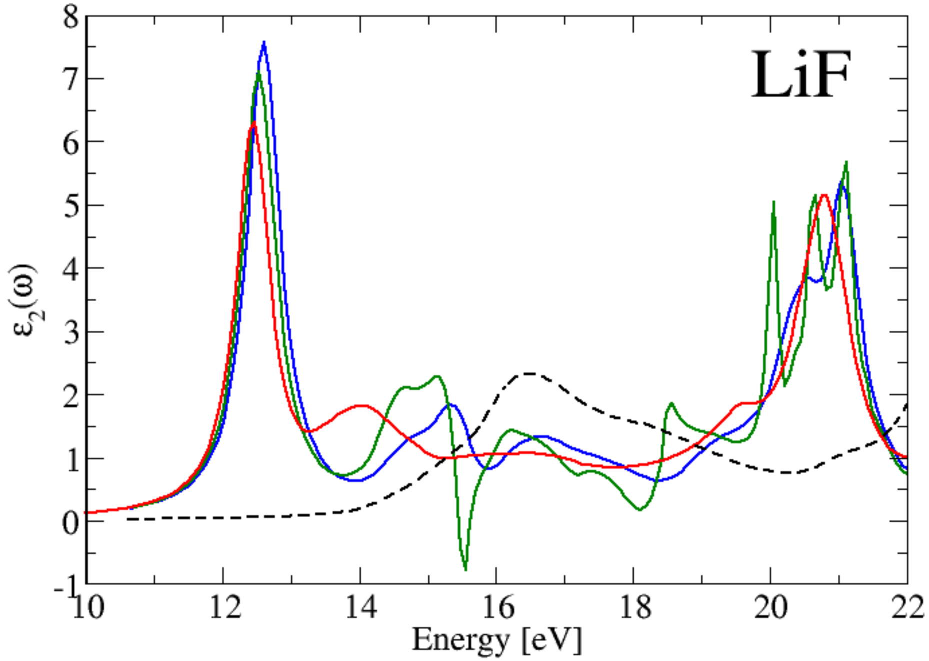
$\mathbf{f}_{xc}^{(2)}(\mathbf{q},\omega) =$ 

$\mathbf{f}_{xc}^{(3)}(\mathbf{q},\omega) =$ 

 $:= \left[\mathbf{P}^{(0)}(\omega)\right]^{-1}$

BSE — — — *QP-RPA*



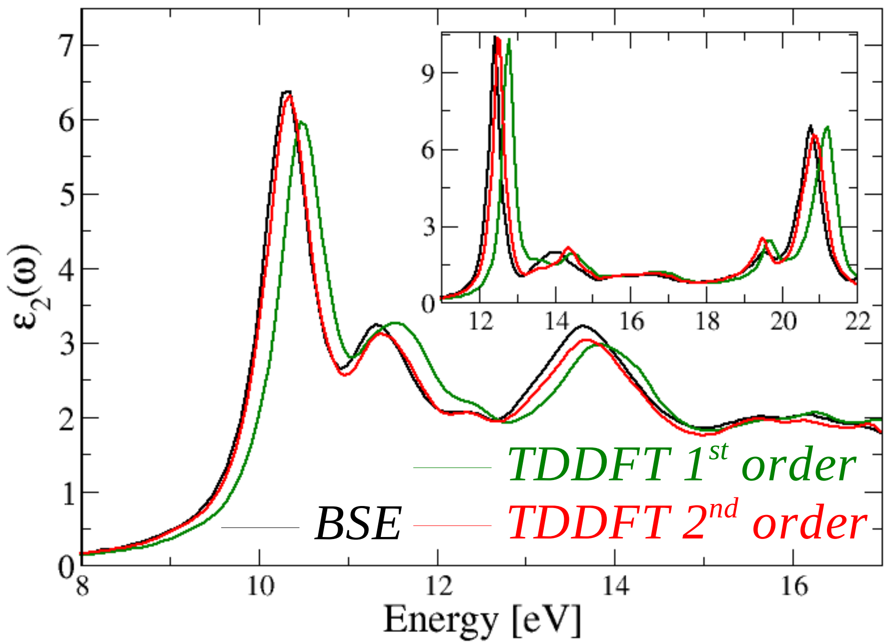


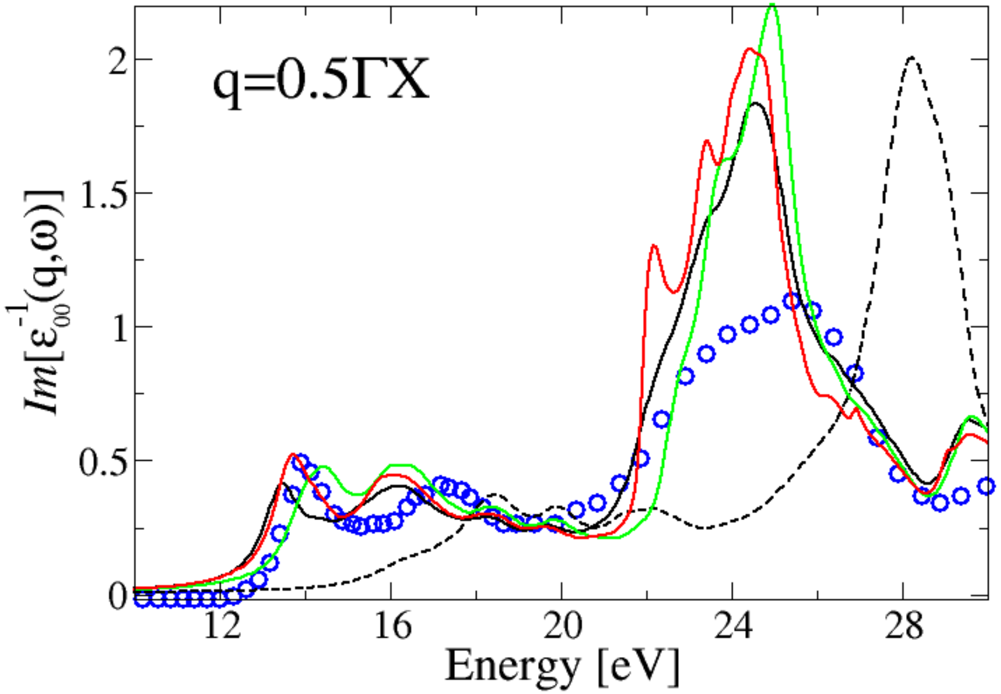
A many-body causal TDDFT kernel

$$\mathbf{f}_{xc}^{(n)}(\mathbf{q},\omega)=\frac{1}{\mathbf{P}^{(0)}(\mathbf{q},\omega)}\left[\delta\tilde{\mathbf{P}}^{(n)}(\mathbf{q},\omega)\left(\mathbf{P}^{(0)}(\mathbf{q},\omega)\right)^{-1}-\sum_{m=1,n-1}(-1)^{m}\,\delta\tilde{\mathbf{P}}^{(m)}(\mathbf{q},\omega)\,\mathbf{f}_{xc}^{(n-m)}(\mathbf{q},\omega)\right]$$

Causal/T-ordered

Causal/T-ordered f_{xc}





- Same agreement between BSE and TDDFT for the finite transferred momentum absorption spectra...
- ...and for the off-diagonal elements of the miscroscopic dielectric function

Low dimensional sytems (1D): polyacetylane

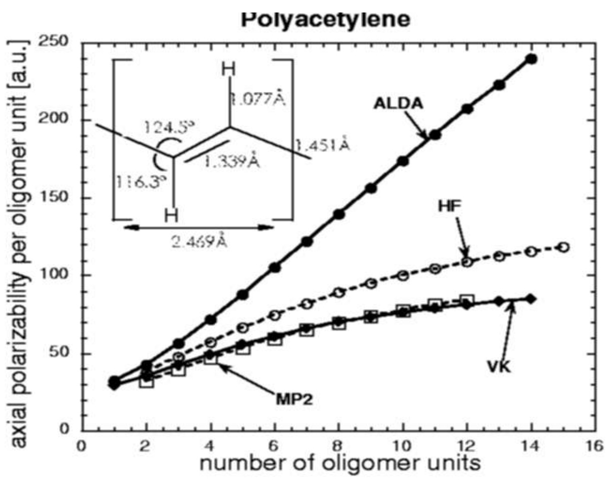


FIG. 1. ALDA and VK static axial polarizability of polyacetylene compared with restricted Hartree-Fock [18] and MP2 [22] results.

M. van Faassen et al. PRL **88** 186401 (2002)

Electric field dependence of the XC Potenital in Molecular Chains

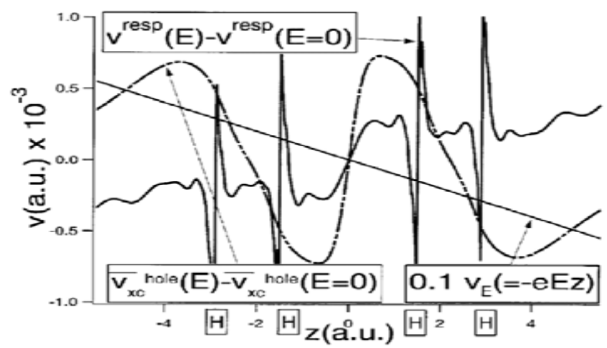


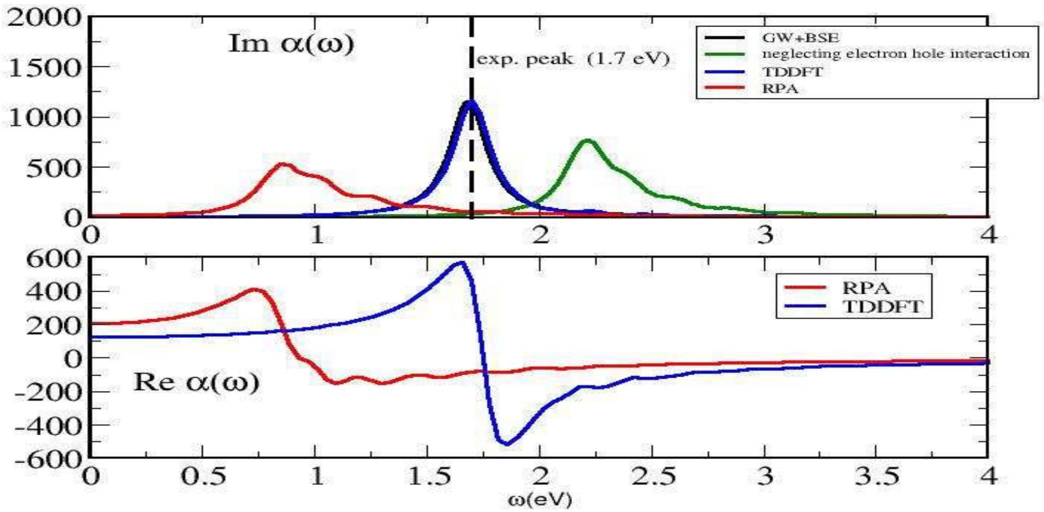
FIG. 2. Changes, due to an electric field of 0.001 a.u. in response and hole potentials for H_2-H_2, constructed from multireference CI singles doubles density with a large (cc-pV6Z without d and f functions) basis set, compared to the applied field (potential v_E).

S.J.A. Van Gisbergen PRL **83** 694 (1999)

In LDA and GGA xc potential lack of a term counteracting the applied electric field

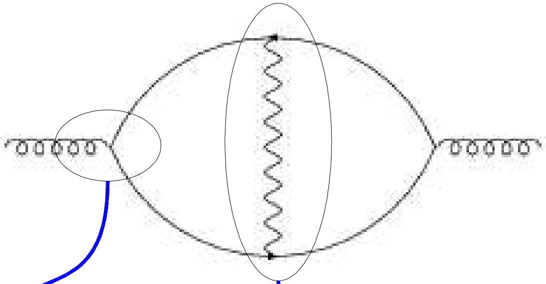
$$f_{xc}^{BSE}(r, r', \omega)$$

Isolated infinite Polyacetylene chain



Is TDDFT "fast" compared to the BSE ?

$$\mathbf{f}_{xc}^{(1)}(\mathbf{q},\omega) =$$



~~[# of frequencies]~~ $\times\, \Phi$ $\times\, W$ $\times\, \Phi'$

$100\, x10000$ $\quad 10000\times 10000$ $\quad 10000\times 100$

$$\mathbf{f}_{xc}^{(1)}(\mathbf{q},\omega) = \frac{2}{\Omega N_k}\left[\mathbf{P}^{(0)}(\mathbf{q},\omega-\Delta_\mathbf{q})\right]^{-1}\sum_{\mathbf{K}}\left[\frac{\mathbf{R}_{\mathbf{K}}^{(\mathbf{q})}+\mathbf{R}_{\mathbf{K}}^{(\mathbf{q})\dagger}}{\omega-E_{\mathbf{K}}^{(\mathbf{q})}-\Delta_\mathbf{q}+i0^+}+\frac{\mathbf{Q}_{\mathbf{K}}^{(\mathbf{q})}}{\left(\omega-E_{\mathbf{K}}^{(\mathbf{q})}-\Delta_\mathbf{q}+i0^+\right)^2}\right]\left[\mathbf{P}^{(0)}(\mathbf{q},\omega-\Delta_\mathbf{q})\right]^{-1}$$

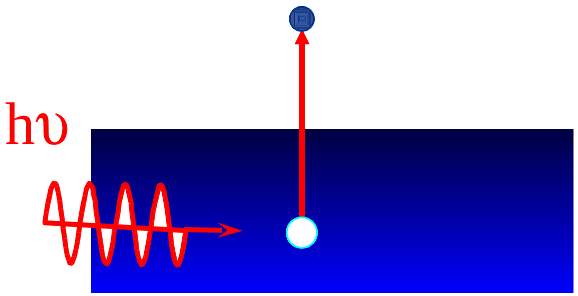
$$\left[R_{\mathbf{K}}^{(\mathbf{q})}\right]_{\mathbf{G}_1,\mathbf{G}_2} = \sum_{\mathbf{K}',E_{\mathbf{K}'}^{(\mathbf{q})}\neq E_{\mathbf{K}}^{(\mathbf{q})}}\frac{\Phi_{\mathbf{K}}^*(\mathbf{q},\mathbf{G}_1)\,W_{\mathbf{K},\mathbf{K}'}(\mathbf{q})\,\Phi_{\mathbf{K}'}(\mathbf{q},\mathbf{G}_2)}{E_{\mathbf{K}}^{(\mathbf{q})}-E_{\mathbf{K}'}^{(\mathbf{q})}} \qquad \left[Q_{\mathbf{K}}^{(\mathbf{q})}\right]_{\mathbf{G}_1,\mathbf{G}_2} = \sum_{\mathbf{K}',E_{\mathbf{K}'}^{(\mathbf{q})}= E_{\mathbf{K}}^{(\mathbf{q})}}\Phi_{\mathbf{K}}^*(\mathbf{q},\mathbf{G}_1)\,W_{\mathbf{K},\mathbf{K}'}(\mathbf{q})\,\Phi_{\mathbf{K}'}(\mathbf{q},\mathbf{G}_2)$$

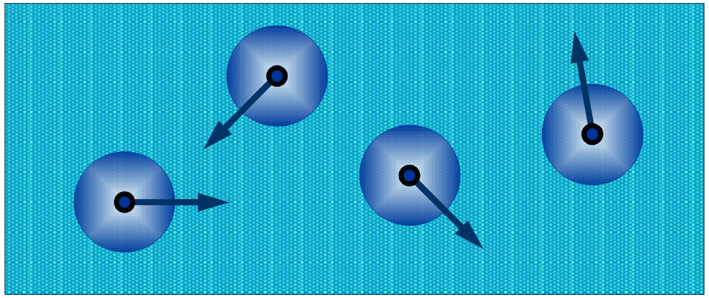
- When the only optical spectra is calculated TDDFT is as time consuming as BSE...
- ...but when the full dielectric matrix is needed TDDFT is more favorable than BSE

What about the description of decaying quasiparticle processes within TDDFT?

G. Onida, L. Reining and AR, Rev. Mod. Phys. ***74****, 601 (2002)*

Lifetime of quasiparticles





interactions between quasiparticles limit how long the corresponding quantum states retain their identity, i.e., the **lifetime** of the excitation.

In combination with the velocity, this lifetime determines the **mean free path**, a measure of influence of the excitation

Importance of lifetime

- screening in an electron gas
- electron-phonon coupling
- localization

surface photochemistry
- electron transfer across interfaces
- electron dynamics and energy transfer

PHYSICS OF LIFETIME

$$\tau^{-1} = 2 \sum \int d\mathbf{r} \int d\mathbf{r}' \, \phi_i^*(\mathbf{r}) \, \phi_f^*(\mathbf{r}') \, \mathrm{Im} W(\mathbf{r},\mathbf{r}';\omega) \, \phi_i(\mathbf{r}') \, \phi_f(\mathbf{r})$$

Density of States (DOS) versus Screening

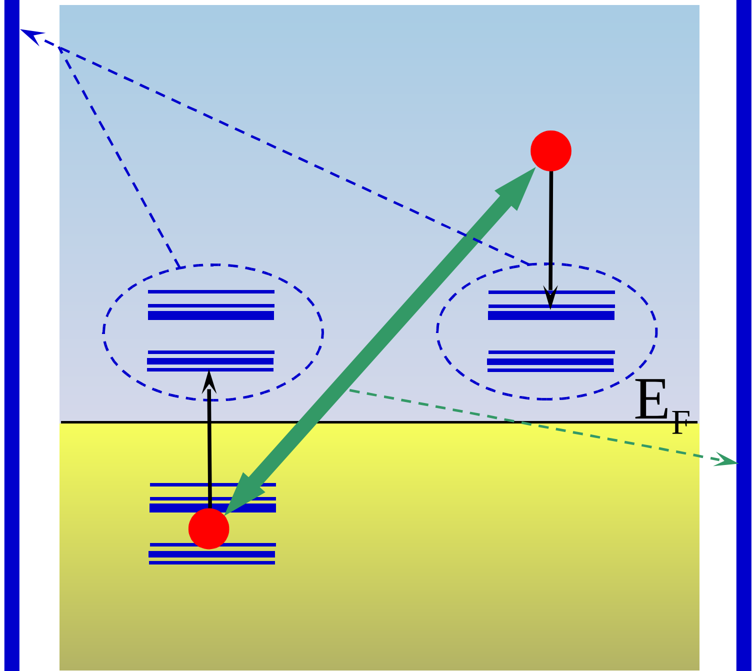
Density of states

More DOS

More phase space available

More probability for the process

Shorter lifetimes



Screening

More DOS

More screening

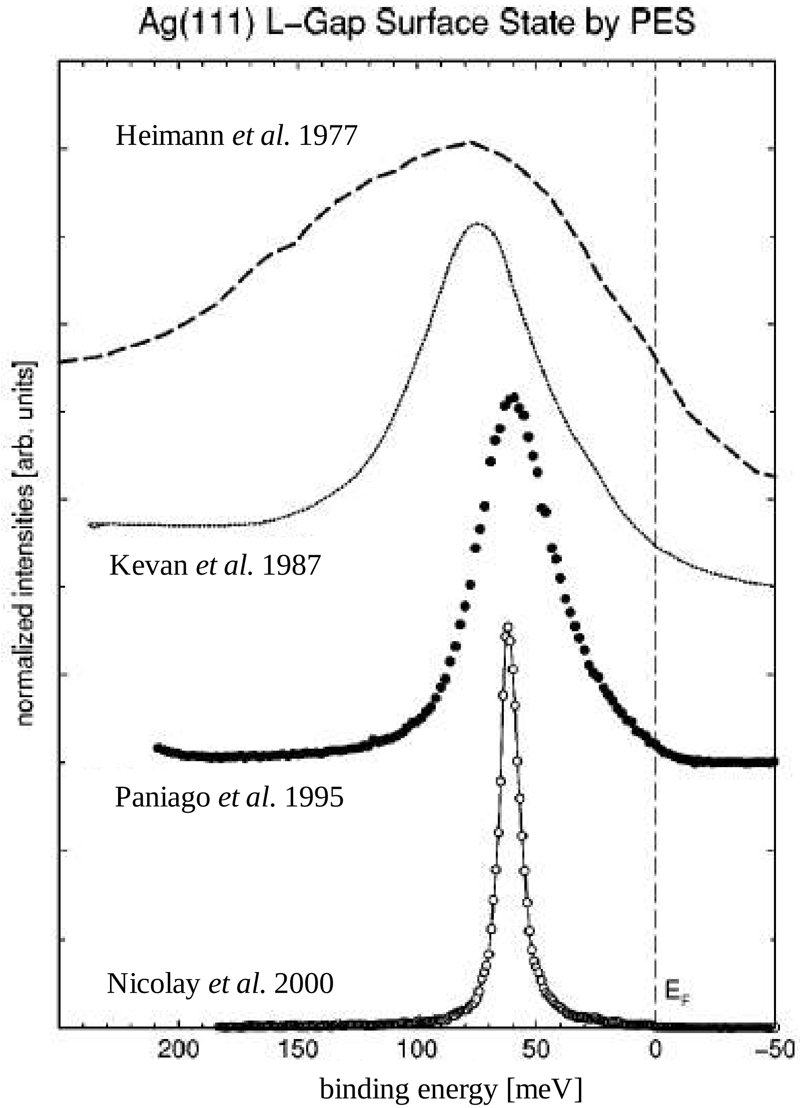
Weaker interaction

Longer lifetimes

Free electrons
Quinn (1962)

$$\tau \approx \frac{263\, r_s^{-5/2}}{(E-E_F)^2} \propto \frac{n^{5/6}}{(E-E_F)^2}$$

Experimental lifetimes change quickly with time!



from F.Reinert *et al.*, PRB **63** (2001) 115415.

The 2-point vertex function

Suppose to have a good approximation fot the (TD)DFT *potential...*

$$\hat{H} = \int d\mathbf{x} \hat{\psi}^{\dagger}(\mathbf{x}) \left[h_0(\mathbf{x}) + v_{xc}(\mathbf{x}) \right] \hat{\psi}(\mathbf{x}) + H_{interaction} - \int d\mathbf{x} \hat{\psi}^{\dagger}(\mathbf{x}) v_{xc}(\mathbf{x}) \hat{\psi}(\mathbf{x})$$

$$\chi(1,2) = \tilde{\chi}(1,2) + \int d34 \tilde{\chi}(1,2) \left[v(3,4) + f_{xc}(3,4) \right] \chi(4,2)$$

$$f_{xc}(1,2) \equiv \delta v_{xc}(1) / \delta \rho(2)$$

$$\tilde{\Gamma}(1,2;3) = \delta(1,2)\delta(2,3) + \int d4567\, \Xi(1,5;2,4) G(4,6) G(7,5) \tilde{\Gamma}(6,7;3)$$

$$\Xi(1,4;2,3) \approx W(1,2)\delta(1,3)\delta(2,4) - f_{xc}(1,3)\delta(1,2)\delta(3,4)$$

$$\Sigma_{G_0W_0} \to i \int d3\, W^{TDDFT}(1^+,3) \tilde{\Gamma}_{loc}(3,2) G(1,2) \qquad \tilde{\Gamma}_{loc}(1,2) = \int d3\, \chi_0^{-1}(1,3) \tilde{\chi}(3,2)$$

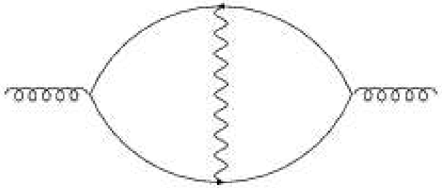
No difference with GoWo using ALDA or similar approaches

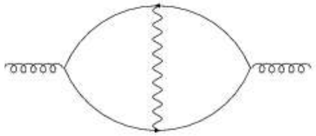
PRL 62, 2718 (1989); PRB 49, 8024 (1994); PRB 56, 12832 (1997).

BUT IS $\tilde{\Gamma}(1,2;3) = \delta(1,2)\delta(2,3) + \tilde{\Gamma}_3(1,2;3) - \tilde{\Gamma}_{loc}(1,3)\delta(1,2) \sim \delta(1,2)\delta(2,3)$ *?*

- *PRL **91**, 056402 (2003);PRL **91**, 256402 (2003). PRL **88**, 066404 (2002) etc etc*

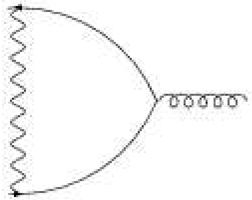
The 3-point vertex function

$\mathbf{f}_{xc}^{(1)}(\mathbf{q},\omega) =$   $:= [\chi_0(\omega)]^{-1}$

$\tilde{\chi}(1,2) = \chi_0(1,2) + \int d34\chi_0(1,3)$  $\tilde{\chi}(4,2) \quad = -i\int d34\, G(1,3)\, G(4,1)\, \widetilde{\Gamma}^{(1)}_{TDDFT}(3,4;2)$

If

$$\widetilde{\Gamma}^{(1)}_{TDDFT}(1,2;3) \equiv \delta(1,2)\,\delta(2,3) + iW_0(1,2)\int d4\, G_0(1,4)\, G_0(4,2)\, \widetilde{\Gamma}_{loc}(4,3)$$

$\widetilde{\Gamma}^{(1)}_{TDDFT}(1,2;3) \equiv \delta(1,2)\,\delta(2,3) + i$  $\tilde{\chi}(4,3)$

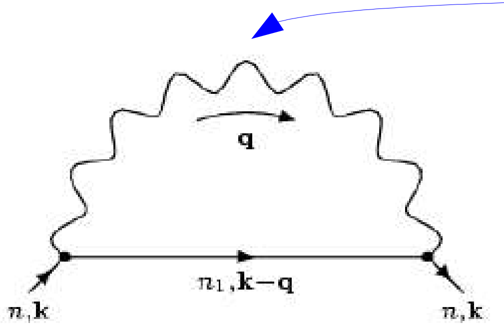
Closed expression for the "on mass-shell" electronic lifetime

$$\tau^{-1}_{c\mathbf{k}} = \tau^{-1}_{c\mathbf{k},0} + \Delta\tau^{-1}_{c\mathbf{k}}$$

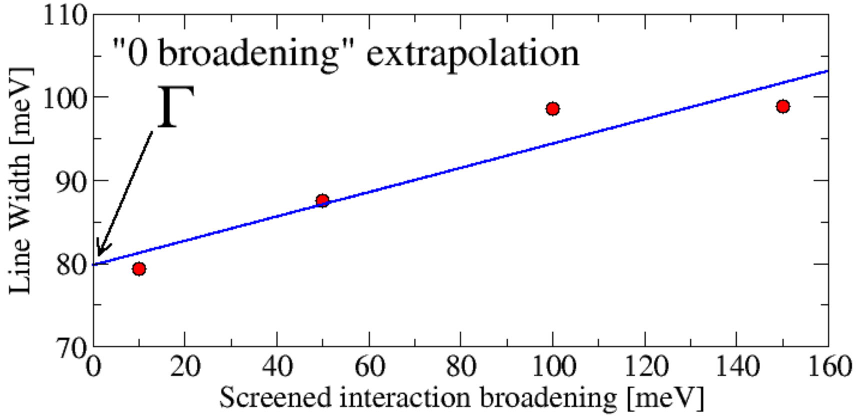
$$\tau^{-1}_{c\mathbf{k},0} = -2\Omega^{-1}\sum_{\mathbf{G}_1,\mathbf{G}_2}\sum_{\mathbf{q},c'} \rho_{cc'}(\mathbf{kqG}_1)\,\rho^*_{cc'}(\mathbf{kqG}_2)\, Im\left[W^{TDDFT}_{\mathbf{G}_1\mathbf{G}_2}(\mathbf{q},\epsilon_{c\mathbf{k}} - \epsilon_{c'\mathbf{k}-\mathbf{q}})\right],$$

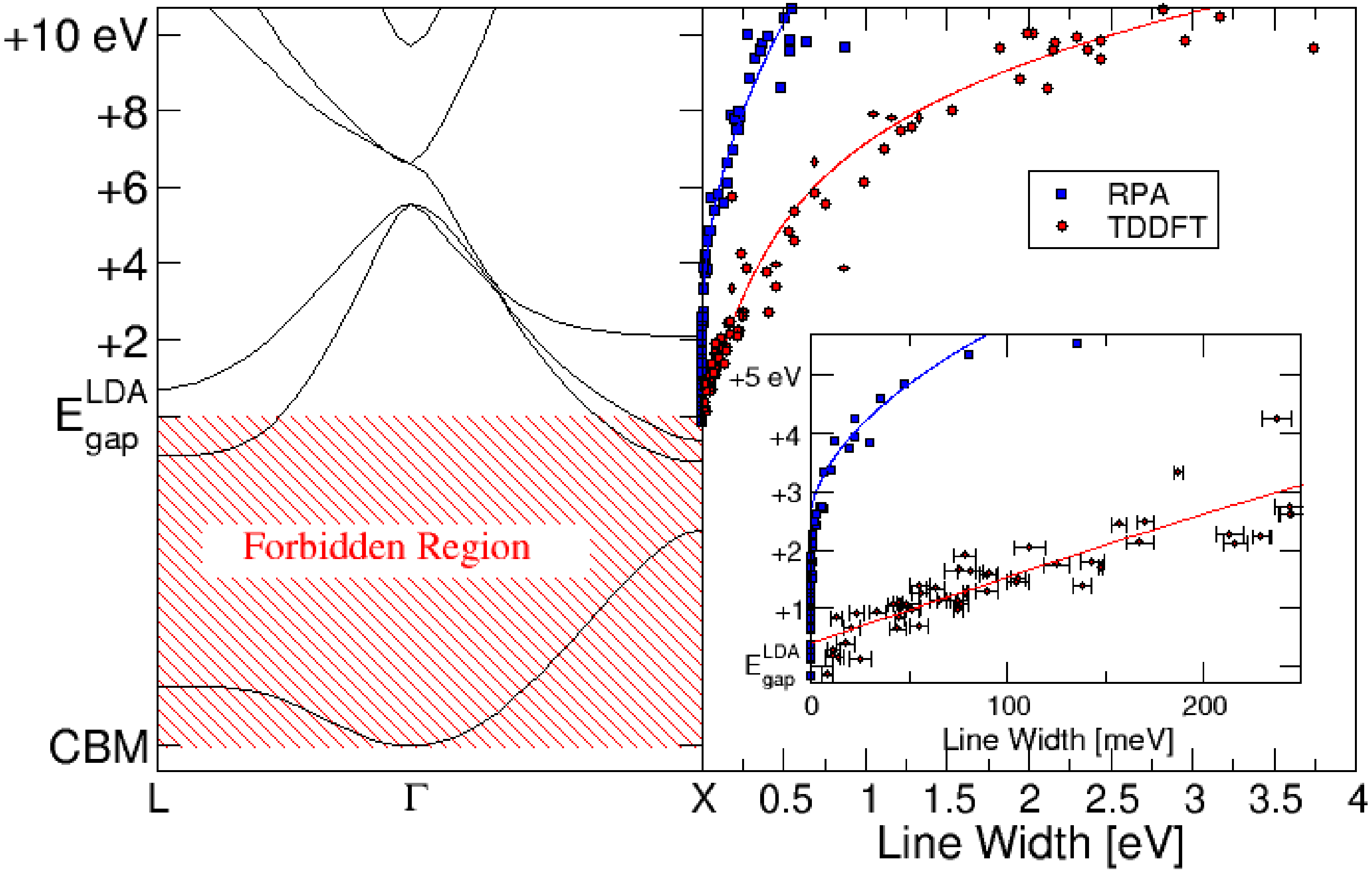
$$\Delta\tau^{-1}_{c\mathbf{k},0} = -2\Omega^{-1}\sum_{\mathbf{G}_1,\mathbf{G}_2}\sum_{\mathbf{q},c'} Re\left[\left(\Gamma^{cv}_{cc'}(\mathbf{kqG}_1) + \Gamma^{vc}_{cc'}(\mathbf{kqG}_1)\right)\rho^*_{cc'}(\mathbf{kqG}_2)\right] Im\left[W^{TDDFT}_{\mathbf{G}_1\mathbf{G}_2}(\mathbf{q},\epsilon_{c\mathbf{k}} - \epsilon_{c'\mathbf{k}-\mathbf{q}})\right]$$

Excitonic effects (via TDDFT) on the lifetimes of LiF



- 10'000x10'000 BS kernel
- Up to 200 G-vectors dielectric function, 256 Q-points in the whole BZ
- Small broadening stability





- Linear behaviour
- Small penetration of the RPA "forbidden region"
- The f_{xc} kernel remains stable and robust even with a 10 meV broadening and energies up to 20 eV
- A BS-based calculation is, in this case, enormously less convenient than using TDDFT

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It is one of the first duties of a professor, in any subject, to exaggerate a little both the importance of his subject and his own importance in it.

G.H. Hardy (A Mathematician's Apology)

Thank you

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