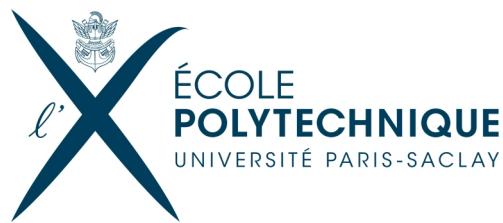


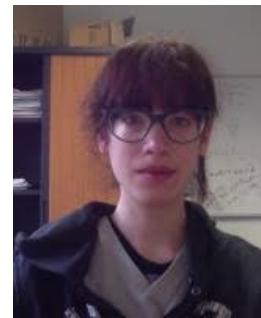
## Palaiseau Theoretical Spectroscopy Group &friends



# Many-body calculations of condensed matter systems



## Palaiseau Theoretical Spectroscopy Group &friends

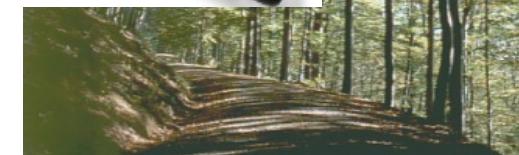
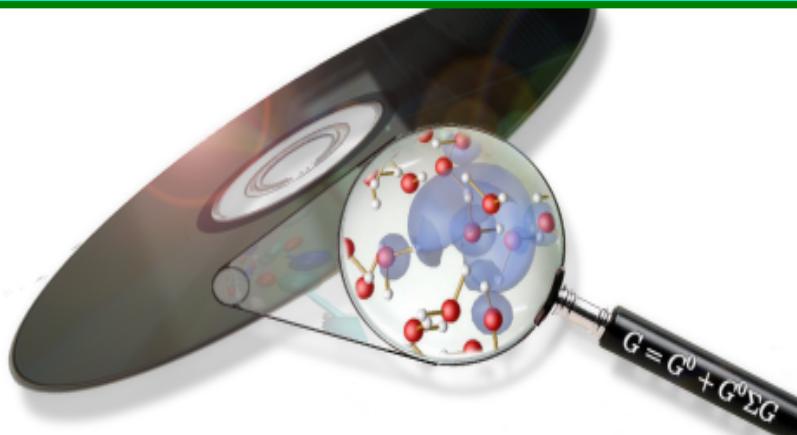
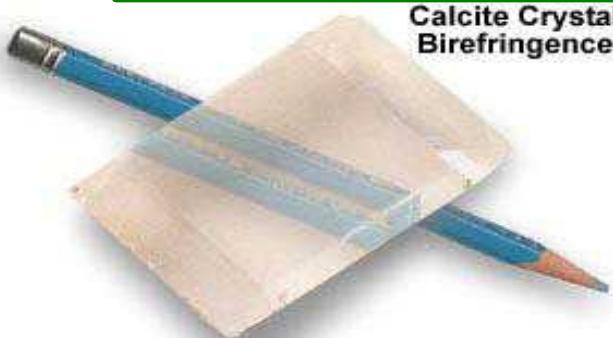


Marco Vanzini  
Jianqiang Sky Zhou  
Ayoub Aouina  
Pierluigi Cudazzo  
Ckaudia Roedl  
Matteo Gatti



Marilena Tzavala  
Martin Panholzer  
John Rehr, Josh Kas (Seattle)

# → Theoretical Spectroscopy: what are we heading for?



→ The framework

→ Recycling I: → Cumulants

- \* *satellites in the one-body spectral function* ✓
- \* *satellites in the two-body spectral function*

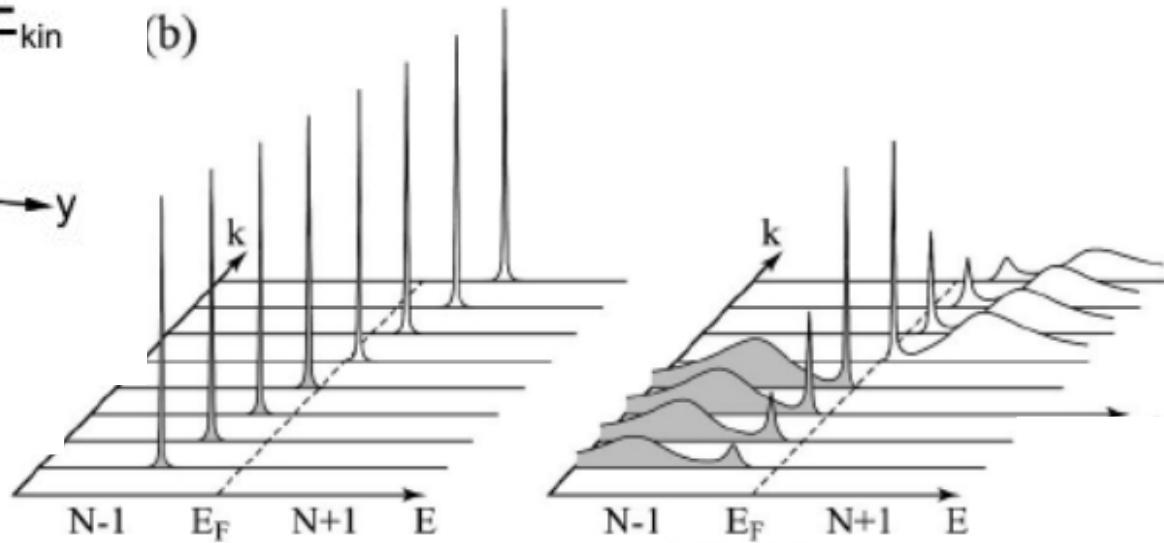
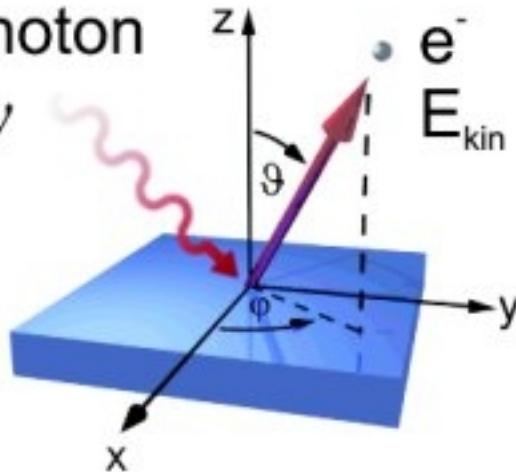
→ Recycling II: → Connector Theory

- \* *the dynamic structure factor* ✓
- \* *the one-body spectral function*

→ Conclusions and outlook

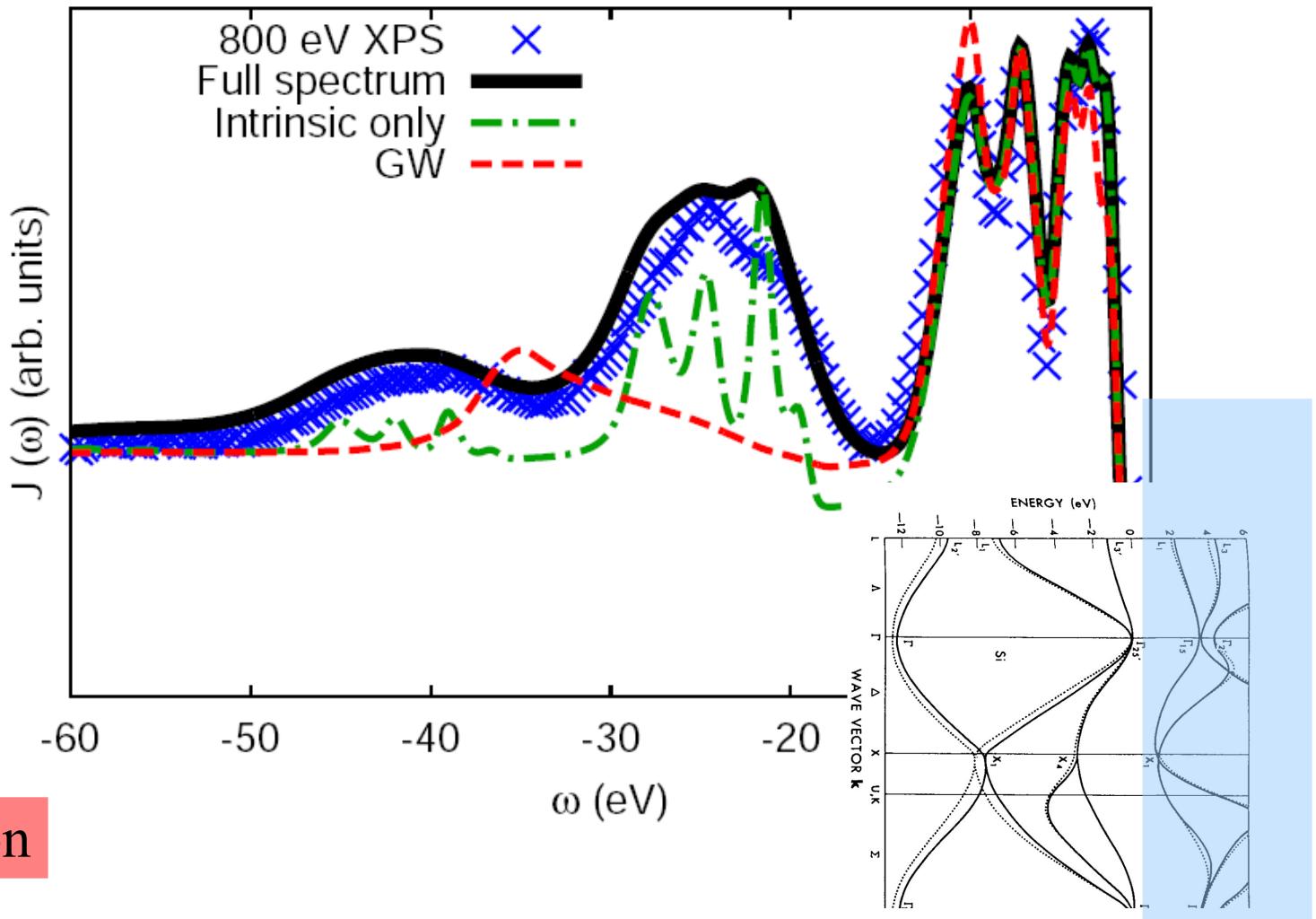
# ARPES

photon  
 $\hbar\nu$



$$A(\omega) \sim \text{Im } G(\omega)$$

*From Damascelli et al., RMP 75, 473 (2003)  
and <http://www.ieap.uni-kiel.de/surface/ag-kipp/arpes/arpes.htm>*



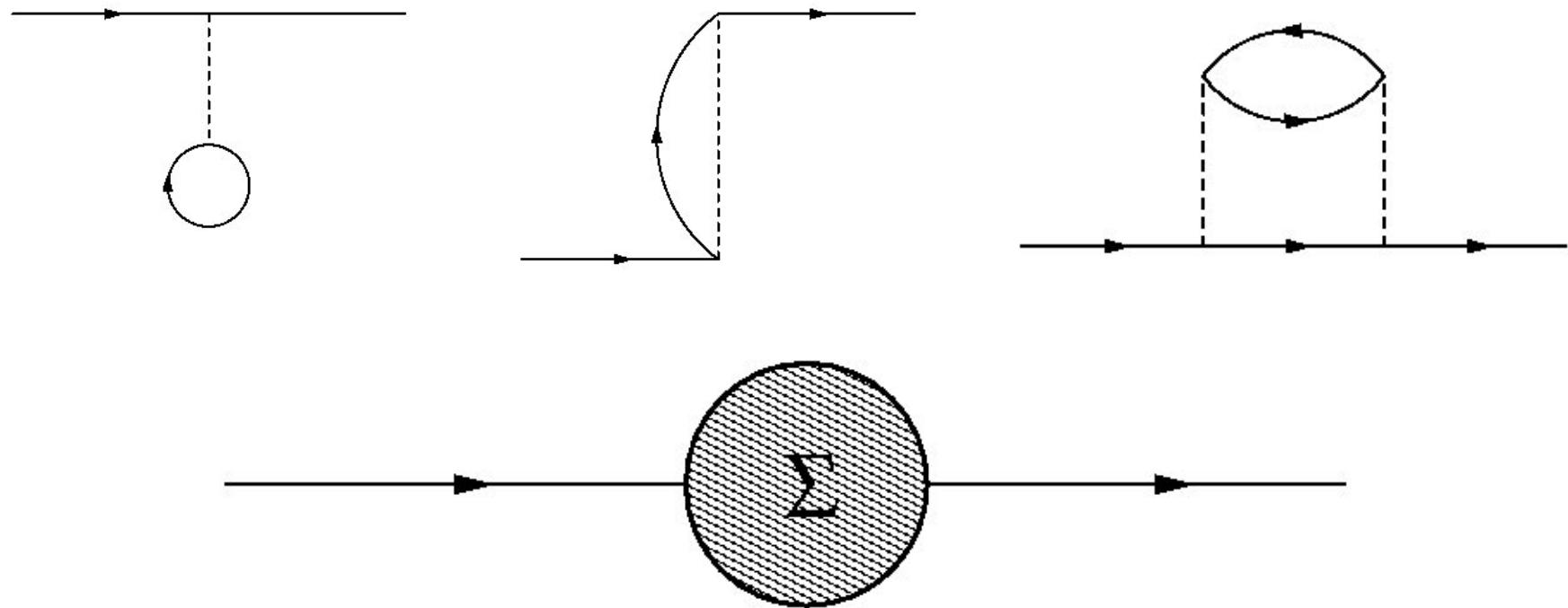
Cohen and Chelikowsky: "Electronic Structure and Optical Properties of Semiconductors" Solid-State Sciences 75, Springer-Verlag 1988)

M. Guzzo et al., PRL 107, 166401 (2011)

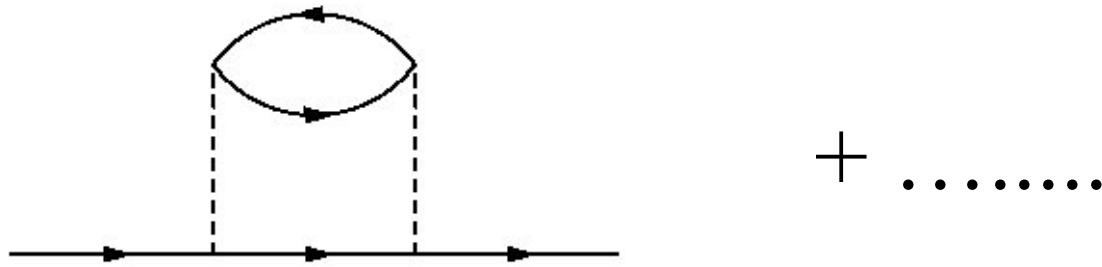
$$G(1, 2) \equiv -i \langle \Psi_0 | \mathbf{T}[\hat{\psi}(1)\hat{\psi}^\dagger(2)] | \Psi_0 \rangle$$

→ The Framework

$$1 = (r_1, \sigma_1, t_1)$$



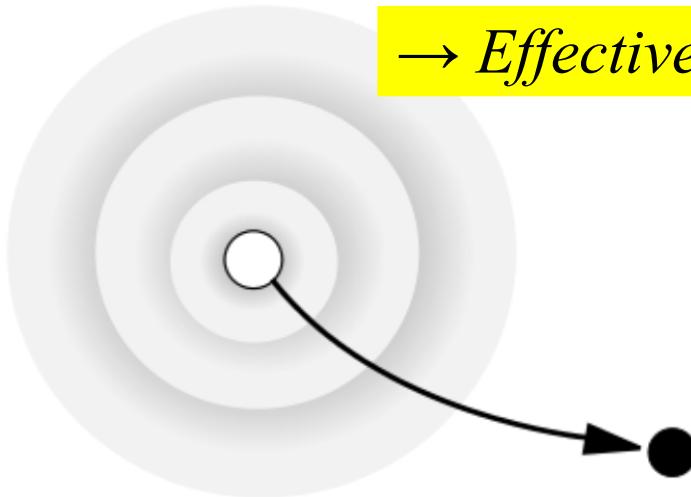
Dyson equation:  $G = G_0 + G_0 \Sigma G$



→  $\Sigma \sim i \mathcal{W}G$  “GW”

L. Hedin (1965)  $W = \varepsilon^{-1}(\omega) v$

→ Effective interaction brings in additional excitations

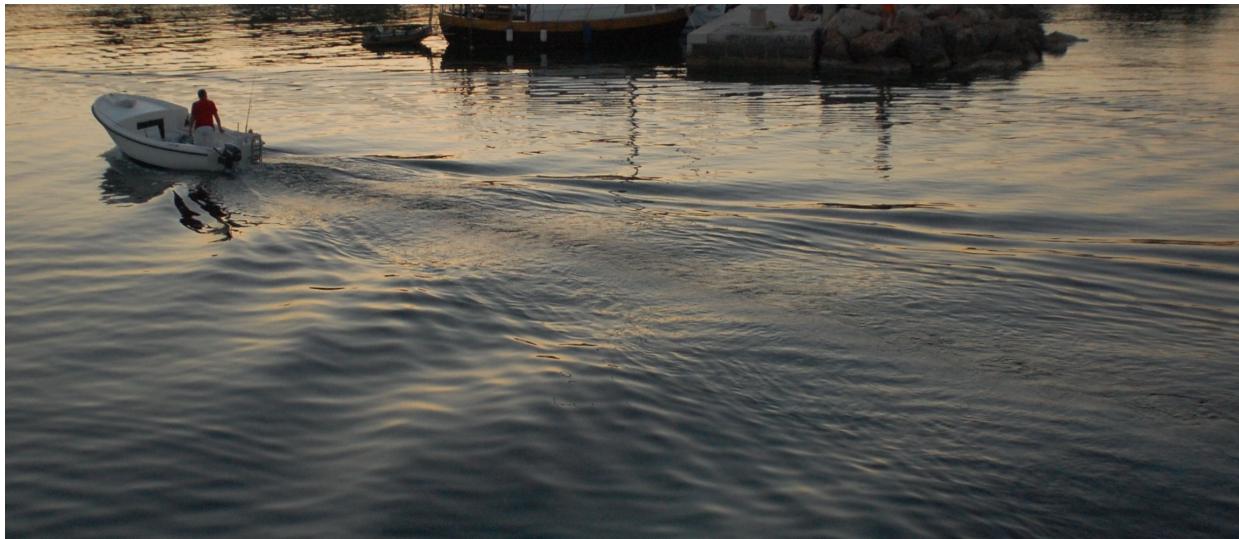


“physical!!!”

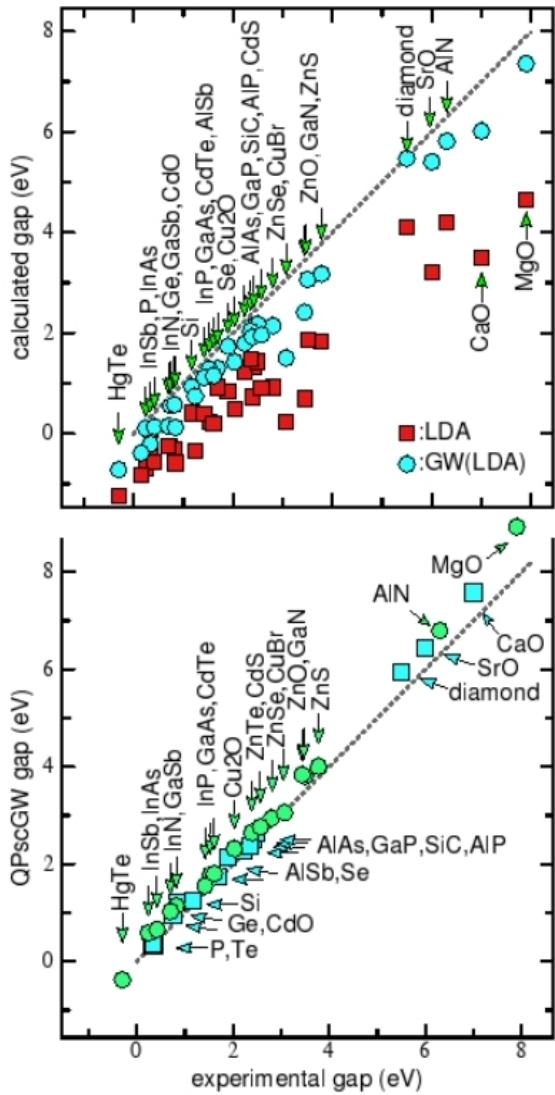
$$\rightarrow \Sigma \sim i \mathcal{W} G \quad \text{“GW”}$$

L. Hedin (1965)

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

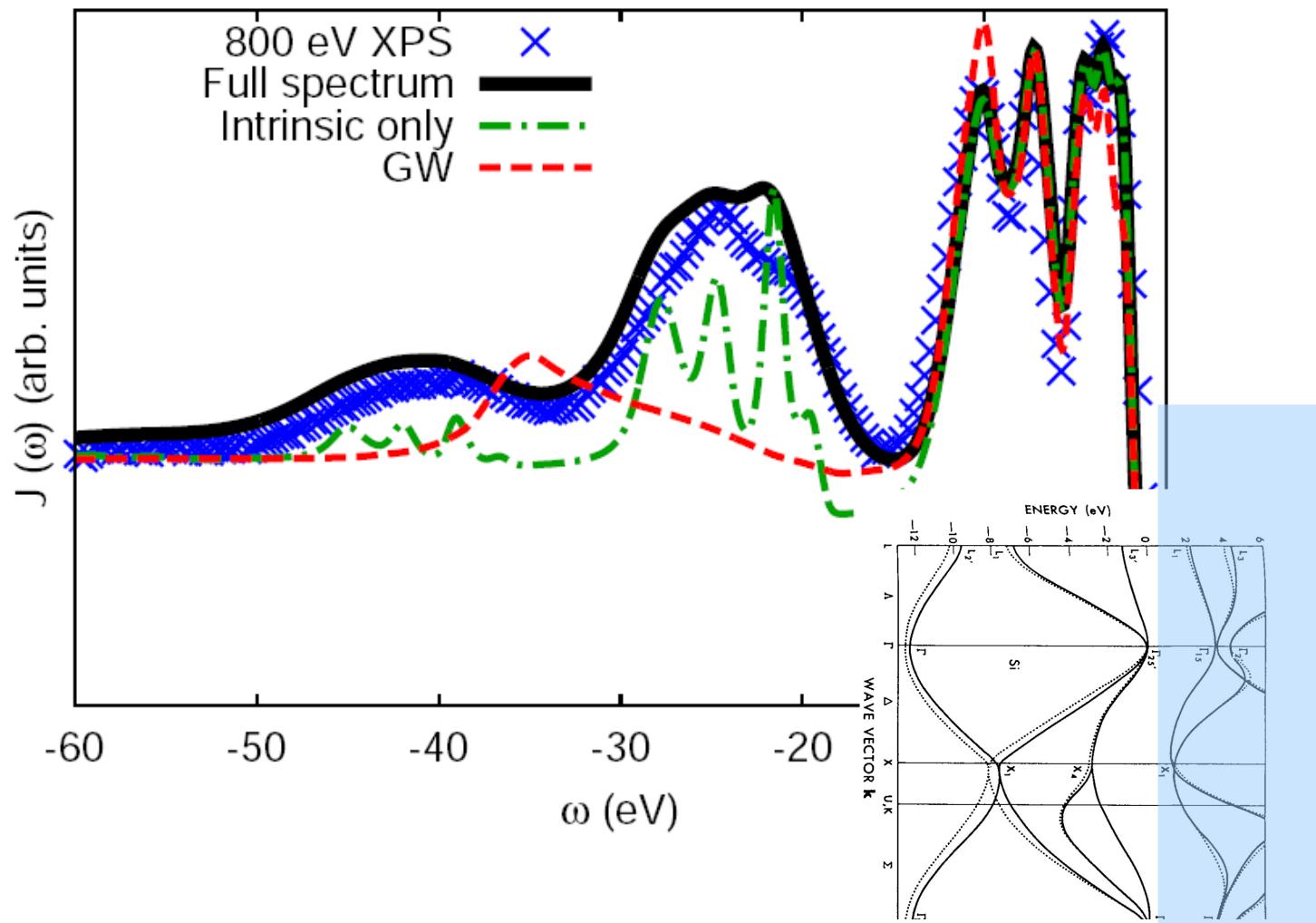


# Usually good gaps and band structures in GW



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

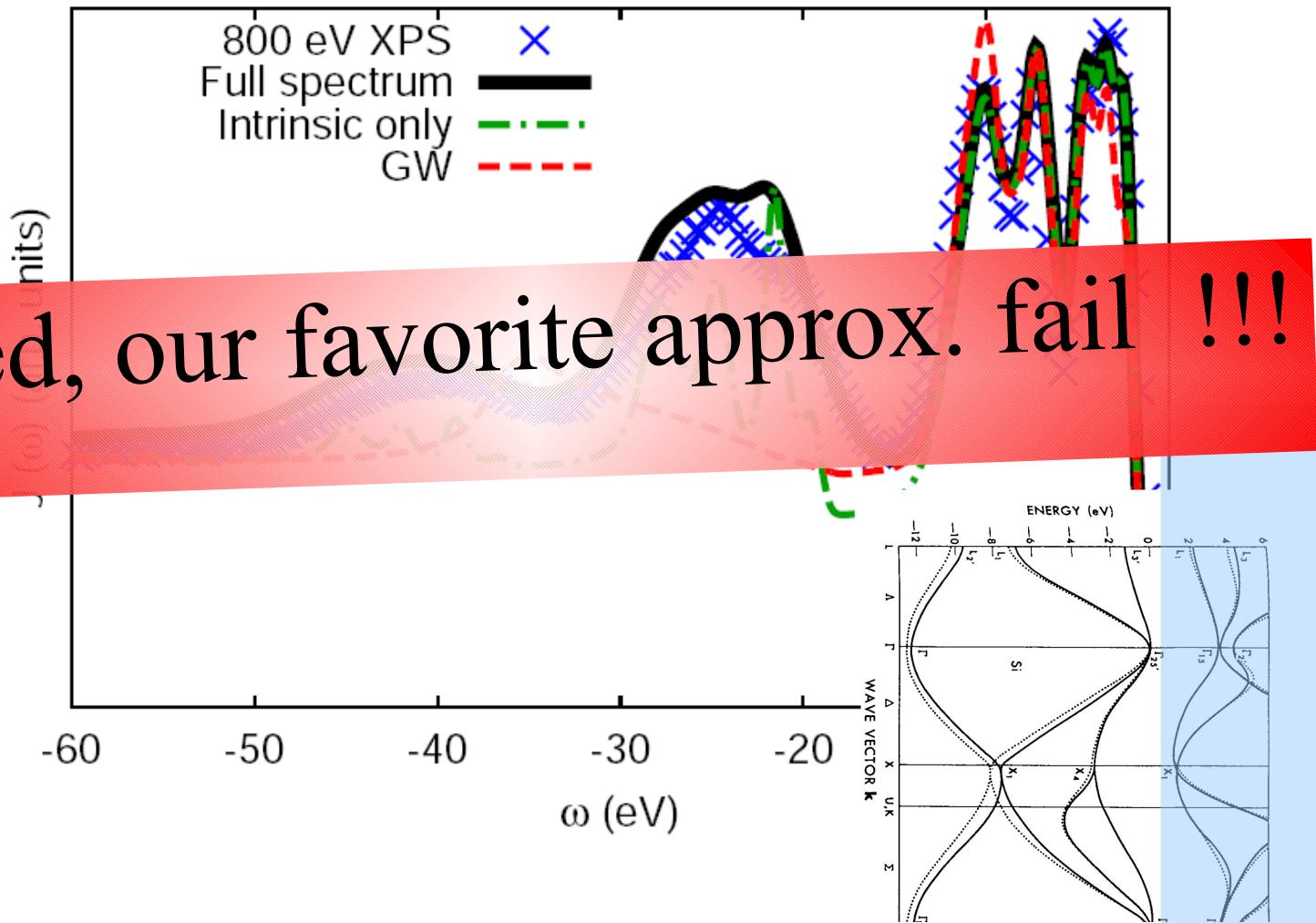
# Self-energy and Satellites



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

M. Guzzo et al., PRL 107, 166401 (2011)

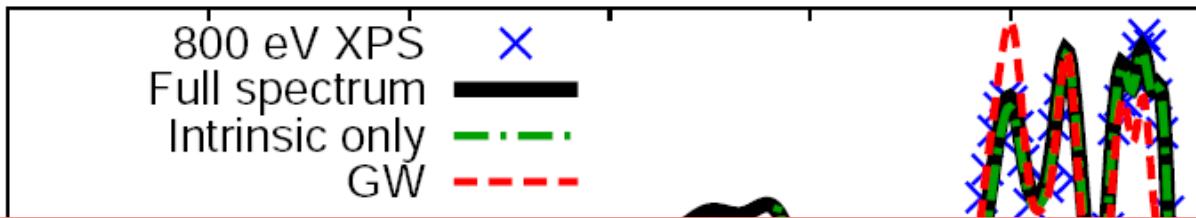
# Self-energy and Satellites



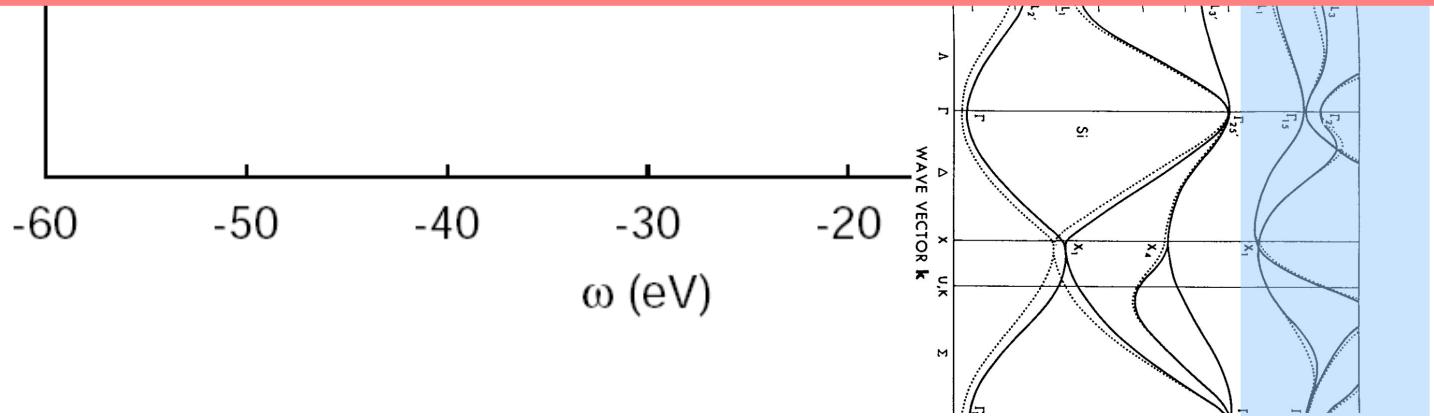
Cohen and Chelikowsky: "Electronic Structure and Optical Properties of Semiconductors" Solid-State Sciences 75, Springer-Verlag 1988)

M. Guzzo et al., PRL 107, 166401 (2011)

# Recycling I: → Cumulants



- Need higher order expressions
- Want many-body also in complex materials
- Try to be more expeditious – or calculate less: recycle!!!



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

M. Guzzo et al., PRL 107, 166401 (2011)

Alternative: solve approximately a functional differential equation

$$G_u(1, 1') = G_{\text{cl}}(1, 1') + iG_{\text{cl}}(1, \bar{2})W_u(\bar{2}, \bar{3})\frac{\delta G_u(\bar{2}, 1')}{\delta u_{\text{cl}}(\bar{3}^+)}$$

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

$$G_{\text{cl}} = G_0 + G_0[U + v_H]G = G_0 + G_0 u_{\text{cl}} G$$

$$1 \equiv (r_1, \sigma_1, t_1)$$

Exact equation that creates diagrams, GW, Hedin's equations,.....

Ansatz:  $G(t_1, t_2) = G_{\text{cl}}(t_1, t_2)\mathcal{F}(t_1, t_2)$

$$G_{ij} = \sum_k G_{\text{cl}}^{ik} \mathcal{F}_{kj}$$

For decoupled orbitals, analytic solution:

$$\mathcal{F}(t_1 - t_2) = \exp \left[ -i \int_{t_1}^{t_2} dt' \int_{t'}^{t_2} dt'' \mathcal{W}(t' t'') \right]$$

$$G_u(1, 1') = G_{\text{cl}}(1, 1') + iG_{\text{cl}}(1, \bar{2})W_u(\bar{2}, \bar{3})\frac{\delta G_u(\bar{2}, 1')}{\delta u_{\text{cl}}(\bar{3}^+)}$$

Exact equation that creates diagrams, GW, Hedin's equations,.....

**Ansatz:**  $G(t_1, t_2) = G_{\text{cl}}(t_1, t_2)\mathcal{F}(t_1, t_2)$

For decoupled orbitals, analytic solution:  $\mathcal{F}(t_1 - t_2) = \exp \left[ -i \int_{t_1}^{t_2} dt' \int_{t'}^{t_2} dt'' \mathcal{W}(t't'') \right]$

With some coupling, still analytic:

$$\mathcal{F}(t_1 - t_2) = \exp \left[ -i \int_{t_1}^{t_2} \text{Linear functional of } \Sigma_{\text{GW}} \right]$$

Recycle GW self-energy to get much improved results!

Note:  $G = \frac{G_{\text{cl}}}{1 - G_{\text{cl}}\Sigma_{\text{xc}}}$  versus  $G = G_{\text{cl}} e^C$

## → Cumulant expansion in bosons

L. Hedin, Physica Scripta **21**, 477 (1980), ISSN 0031-8949.

L. Hedin, J. Phys.: Condens. Matter **11**, R489 (1999).

P. Nozieres and C. De Dominicis, Physical Review **178**, 1097 (1969), ISSN 0031-899X.

D. Langreth, Physical Review B **1**, 471 (1970).

**Sodium: Aryasetiawan et al., PRL 77, 1996**

**Silicon: Kheifets et al., PRB 68, 2003**

**In DMFT context: Casula, Rubtsov, Biermann, PRB 85, 035115 (2012)**

Here:

- the first in a series of approximations
- link to GW
- prescription for ingredients

→ Electron-boson coupling

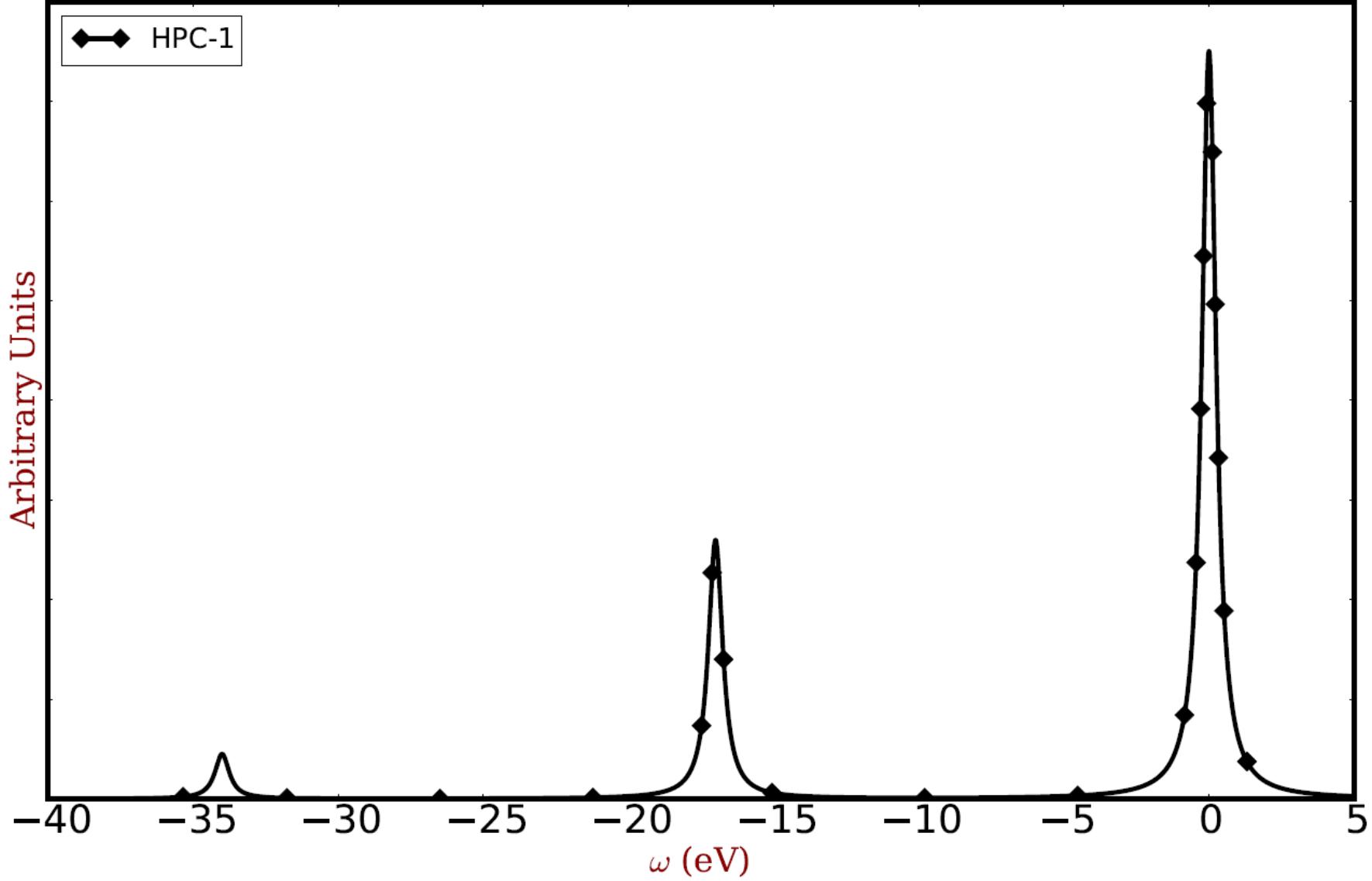
$$H = \epsilon_0 c^\dagger c + cc^\dagger g(a + a^\dagger) + \omega_0 a^\dagger a$$

$$A^h(\omega) = \sum_{n=0}^{\infty} \frac{\beta^n e^{-\beta}}{n!} \delta(\omega - \epsilon_0 - \beta\omega_0 - n\omega_0)$$

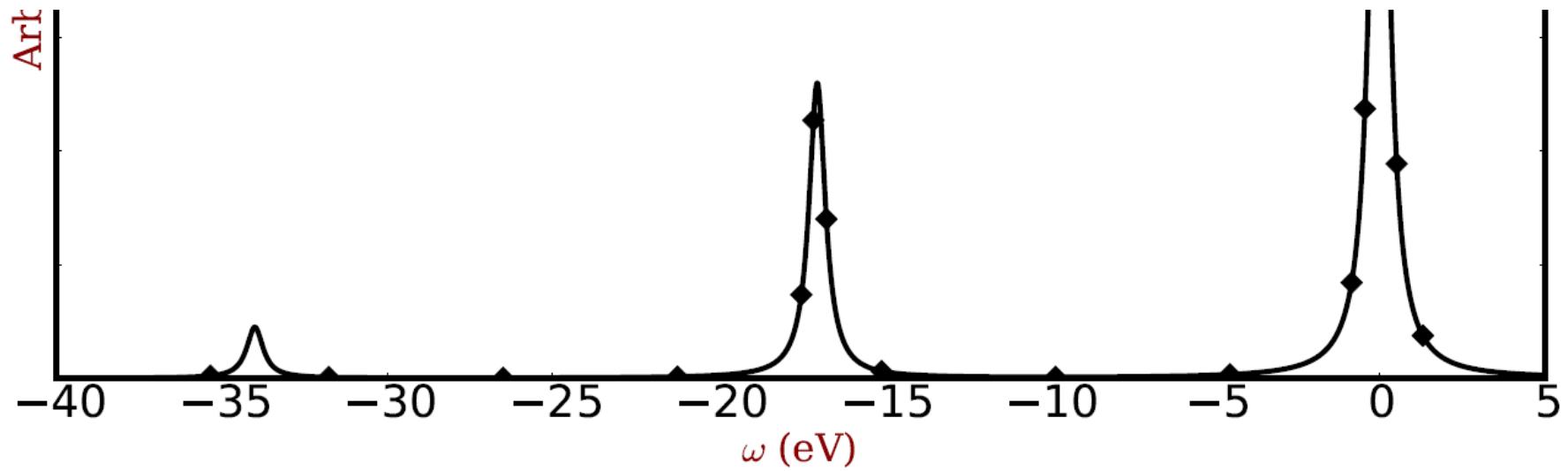
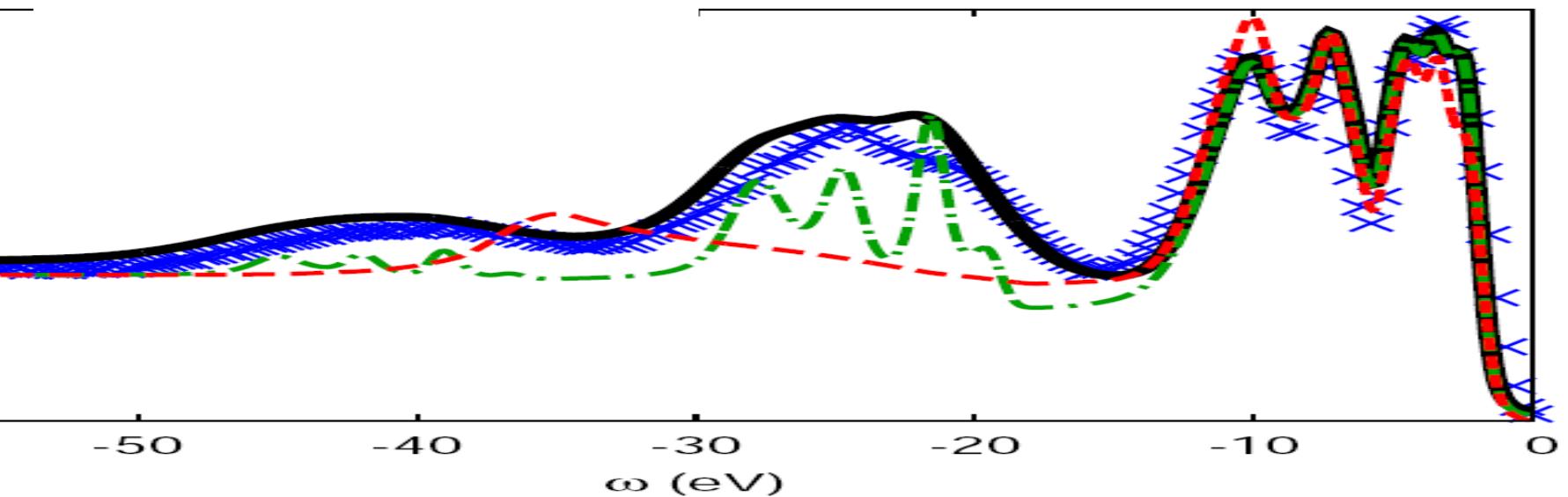
$$\beta = \frac{g^2}{\omega_0^2}$$

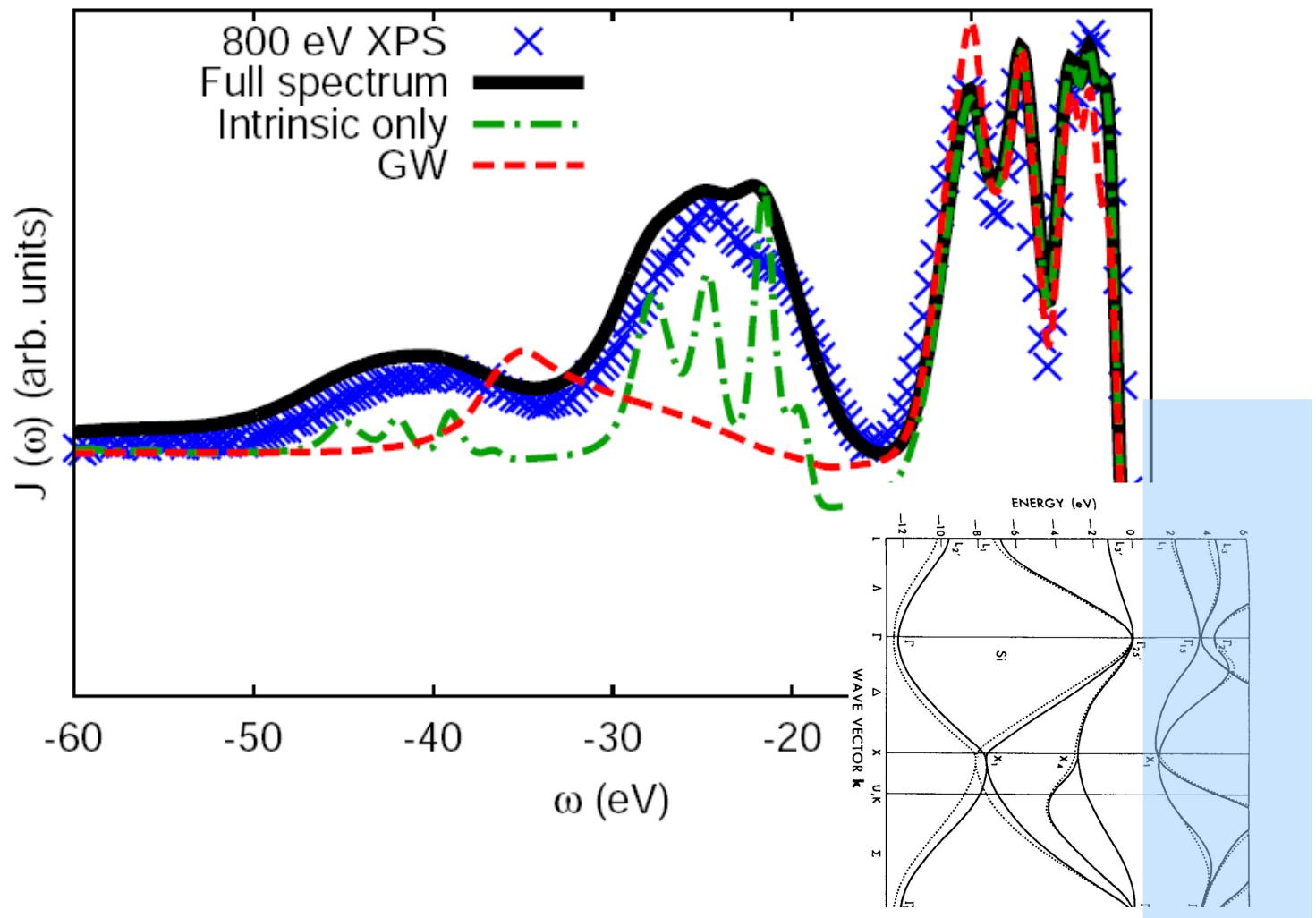
Very general!

# Silicon



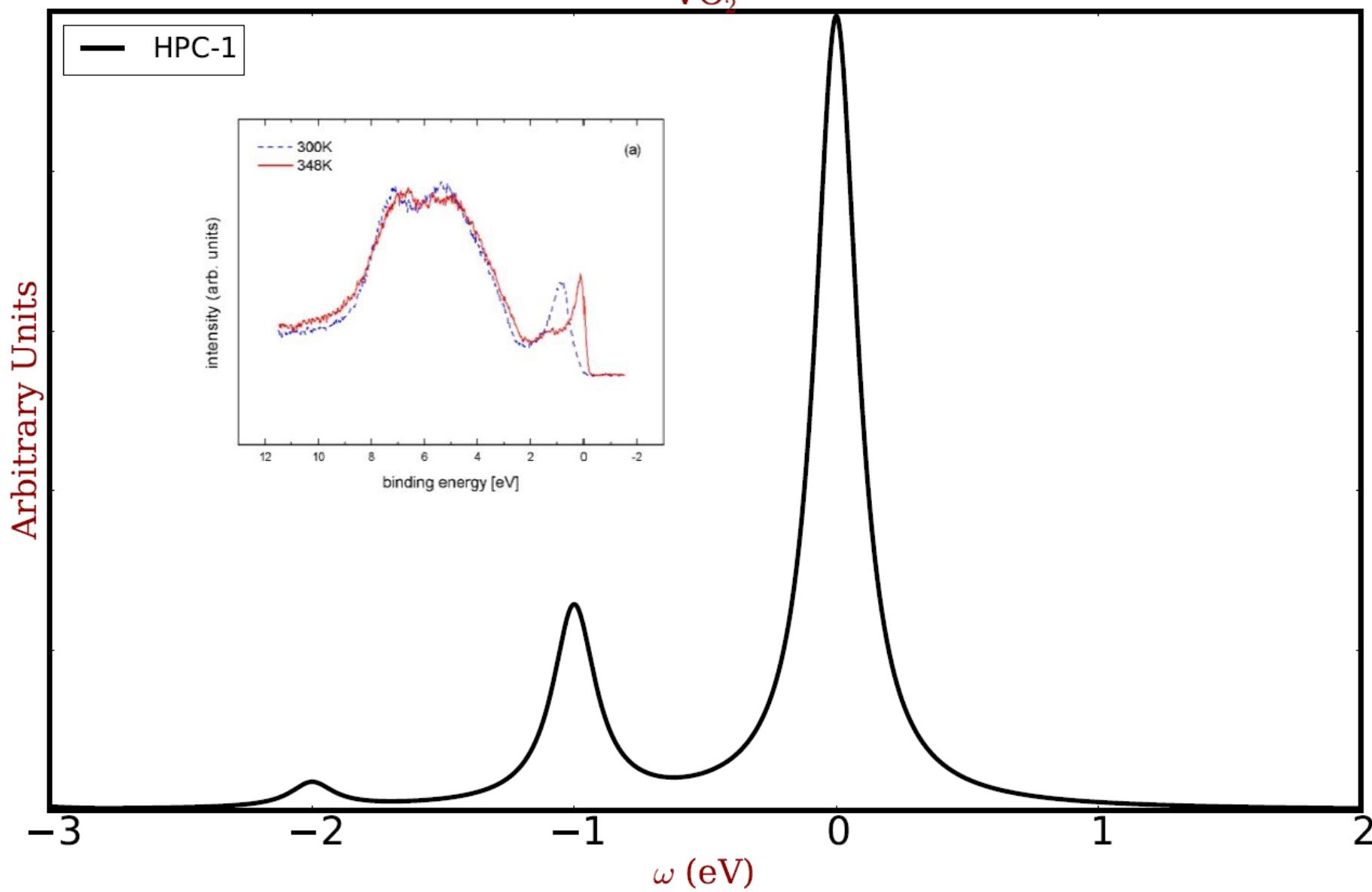
Silicon



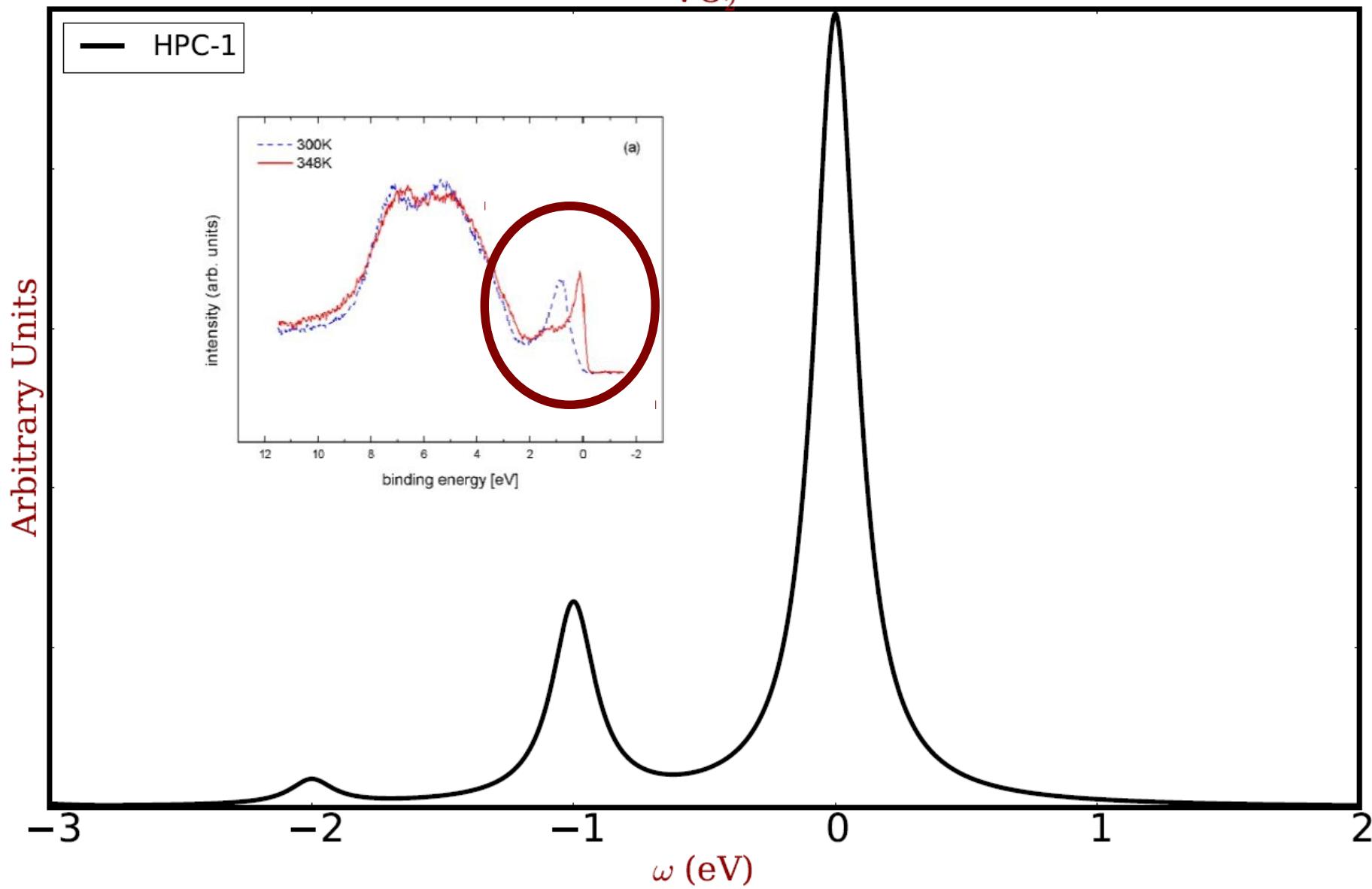


Exp.: F. Sirotti et al., TEMPO beamline SOLEIL

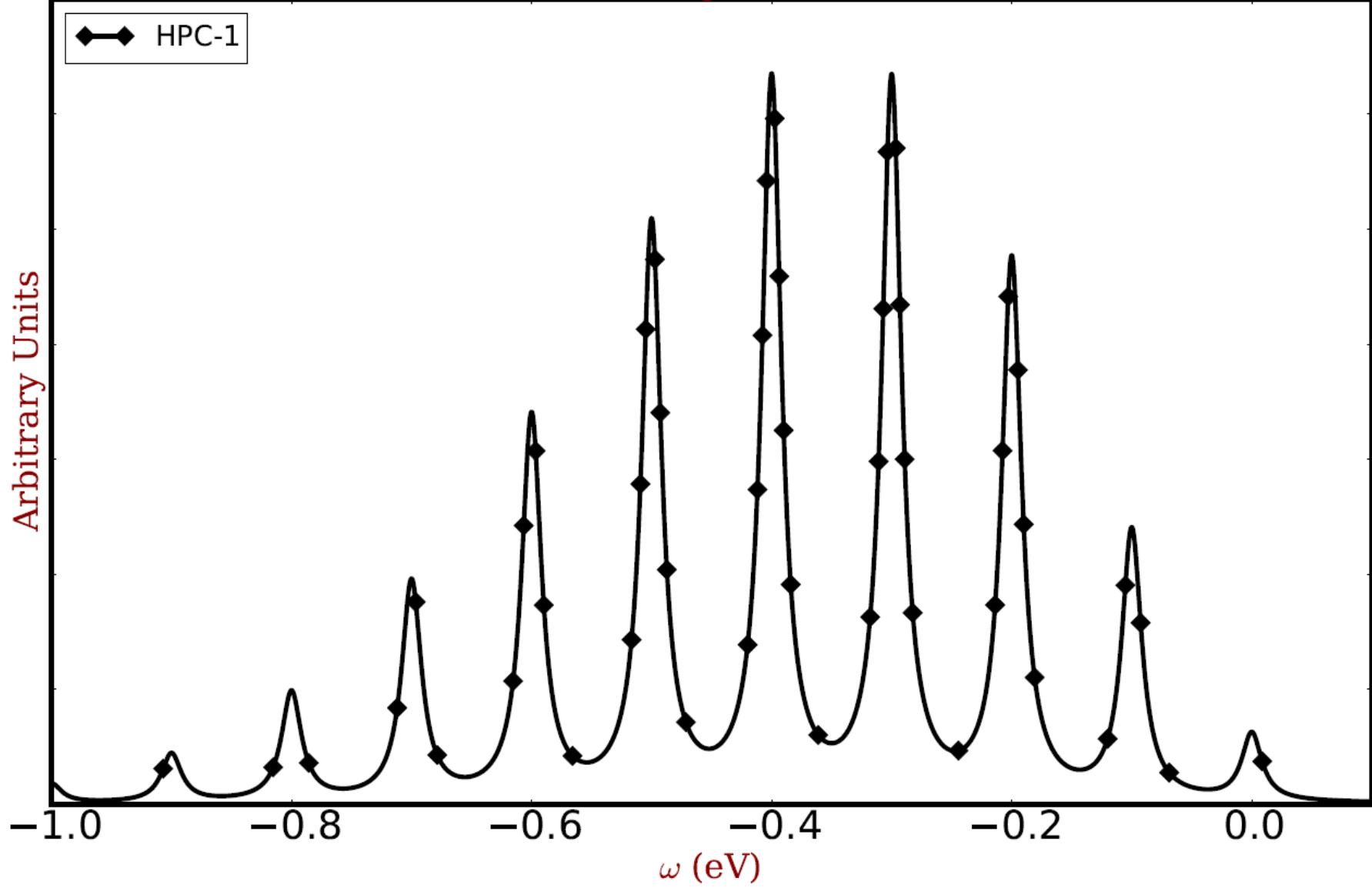
VO2



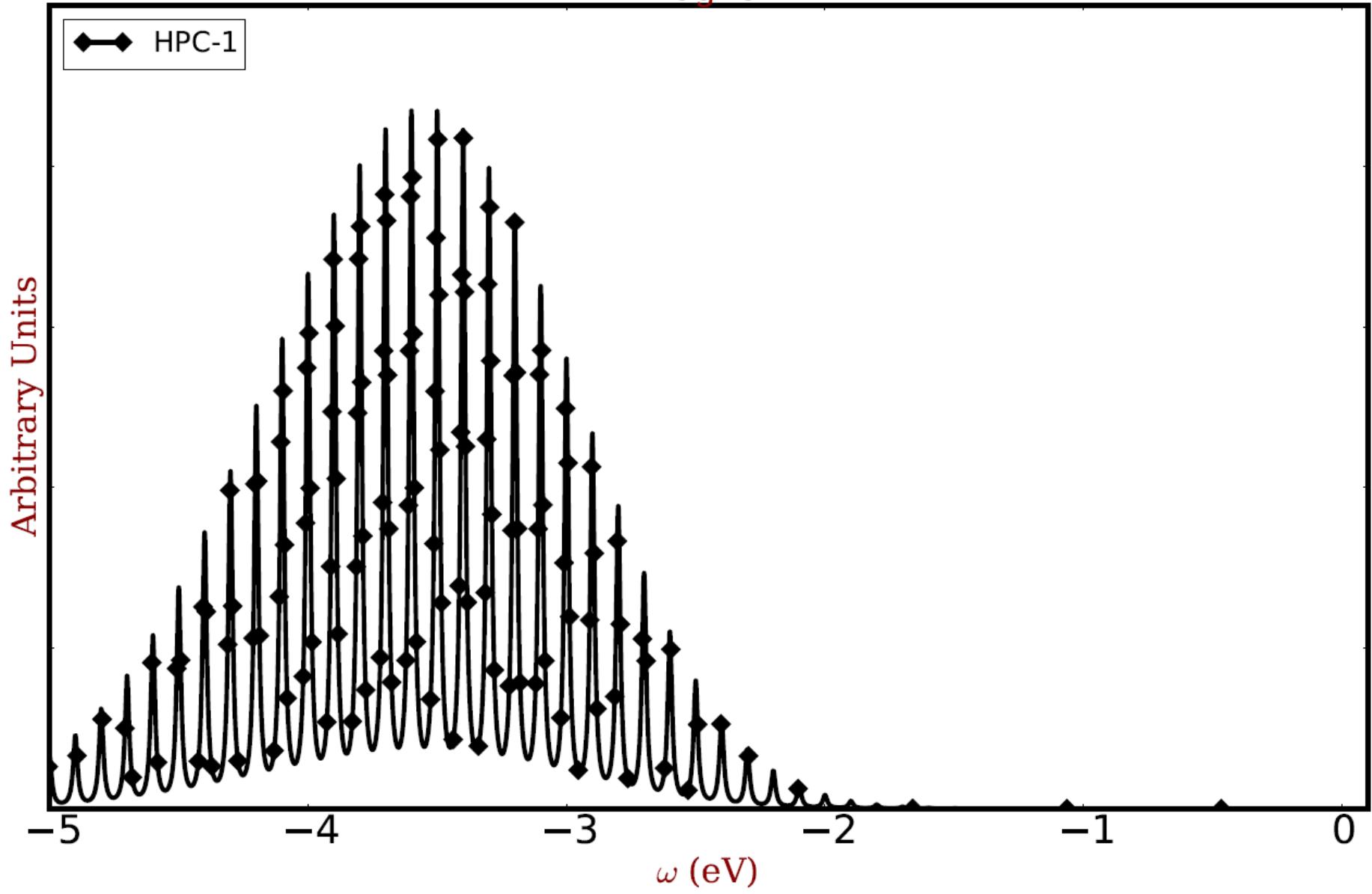
$\text{VO}_2$



# Magnon

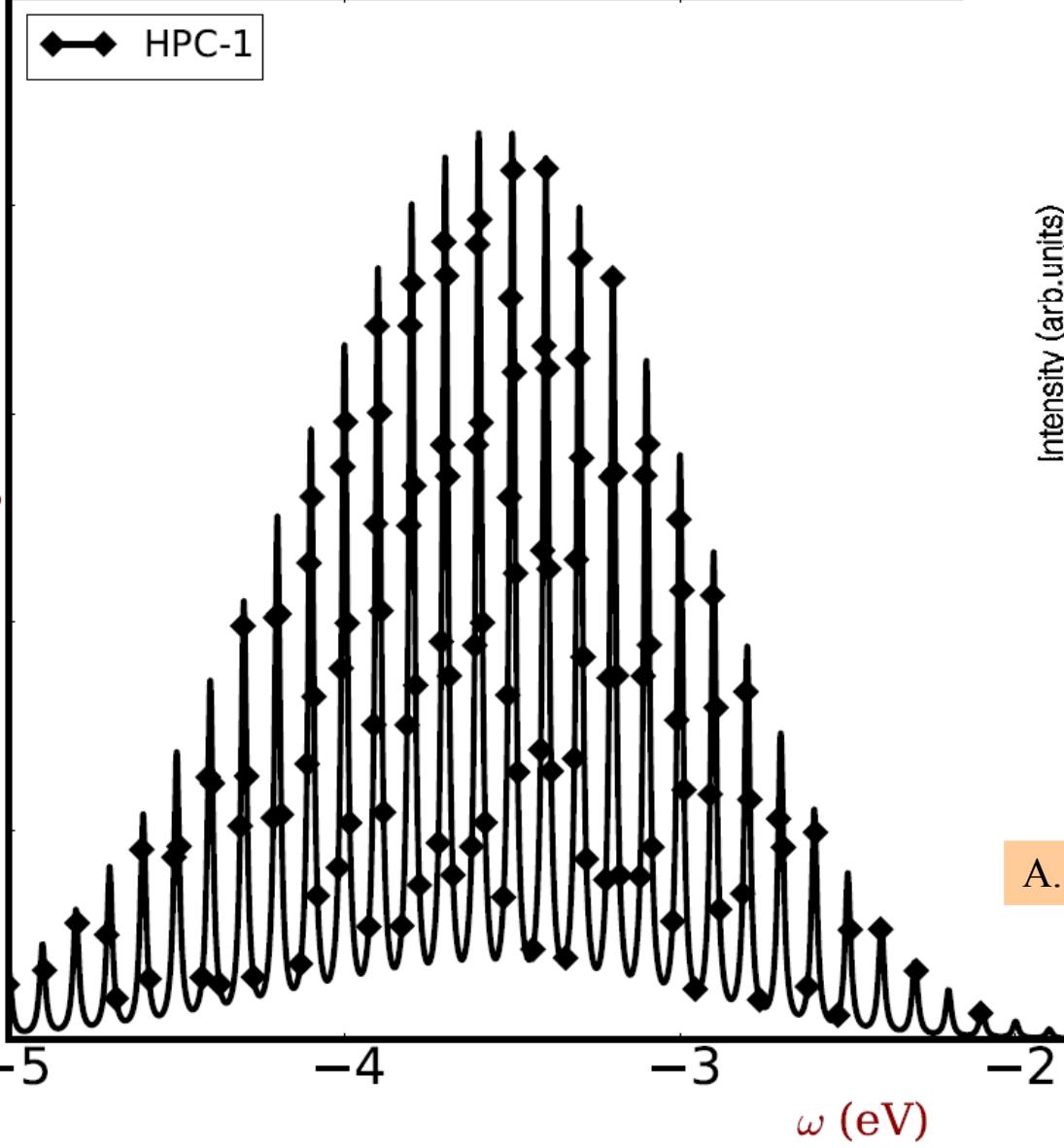


# Magnon

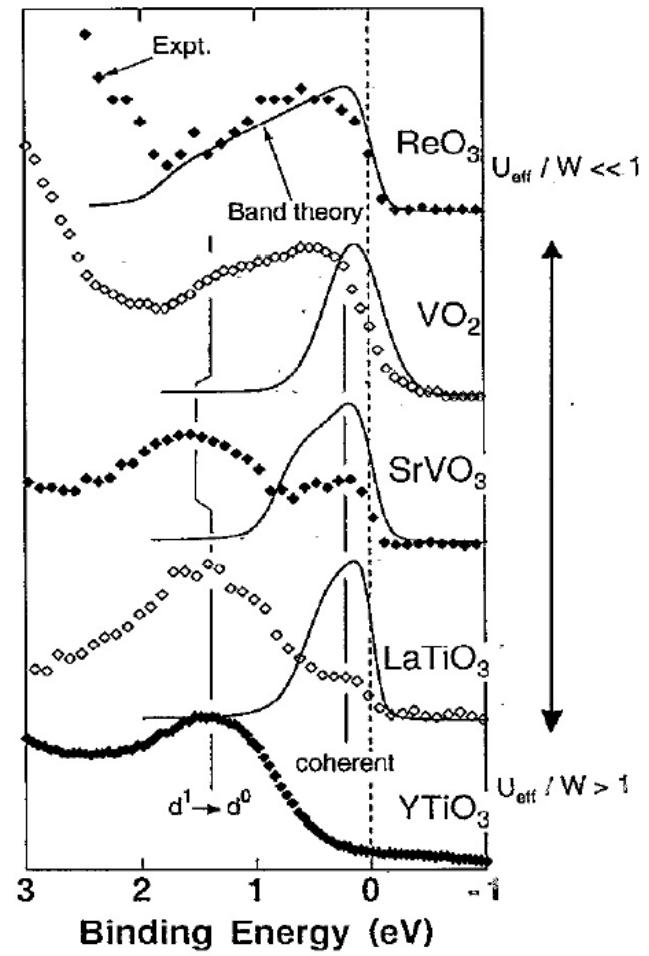


## Magnon

Arbitrary Units



◆◆ HPC-1



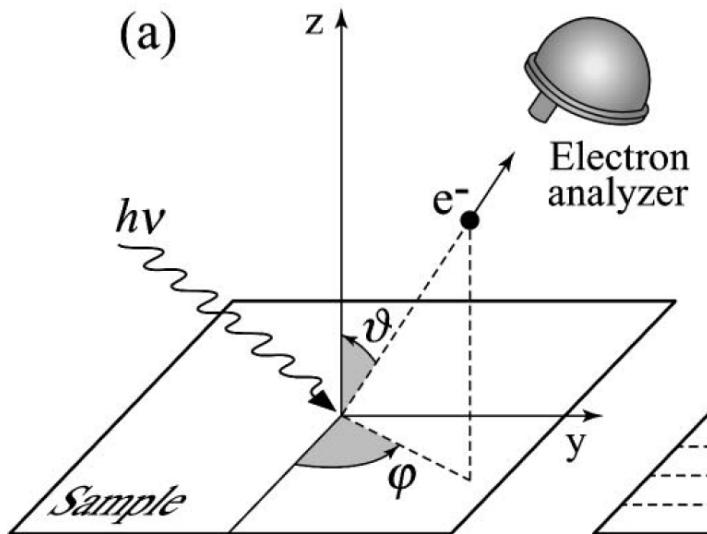
A. Fujimori et al., PRL 69, 1796 (1992)

Convincing description in terms of electron-boson coupling....

IF

- we solve the coupled problem reasonably well
- we have the boson (plasmon, magnon, photon, phonon,...)

(a)



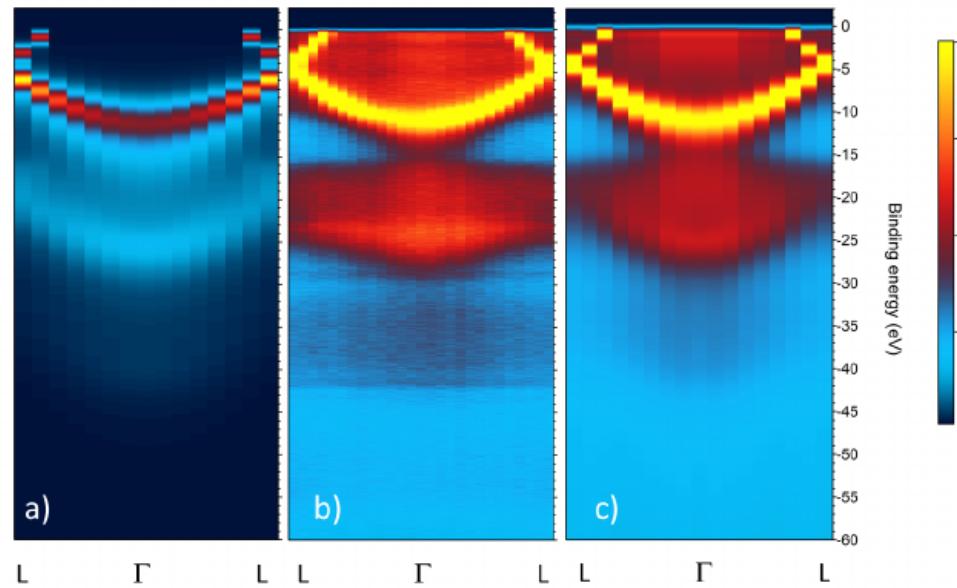
ARPES bulk aluminum

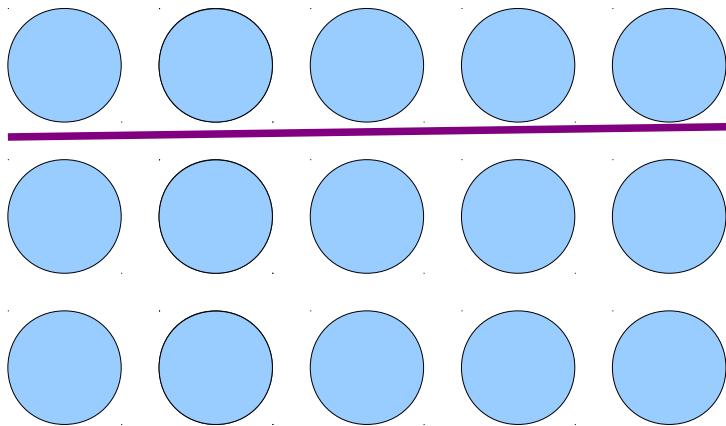
Exp.: Swiss Light Source

Zhou, Reining, Nicolaou, Bendounan, Ruotsalainen, Vanzini, Kas, Rehr, Muntwiler, Strocov, Sirotti, Gatti, 2018



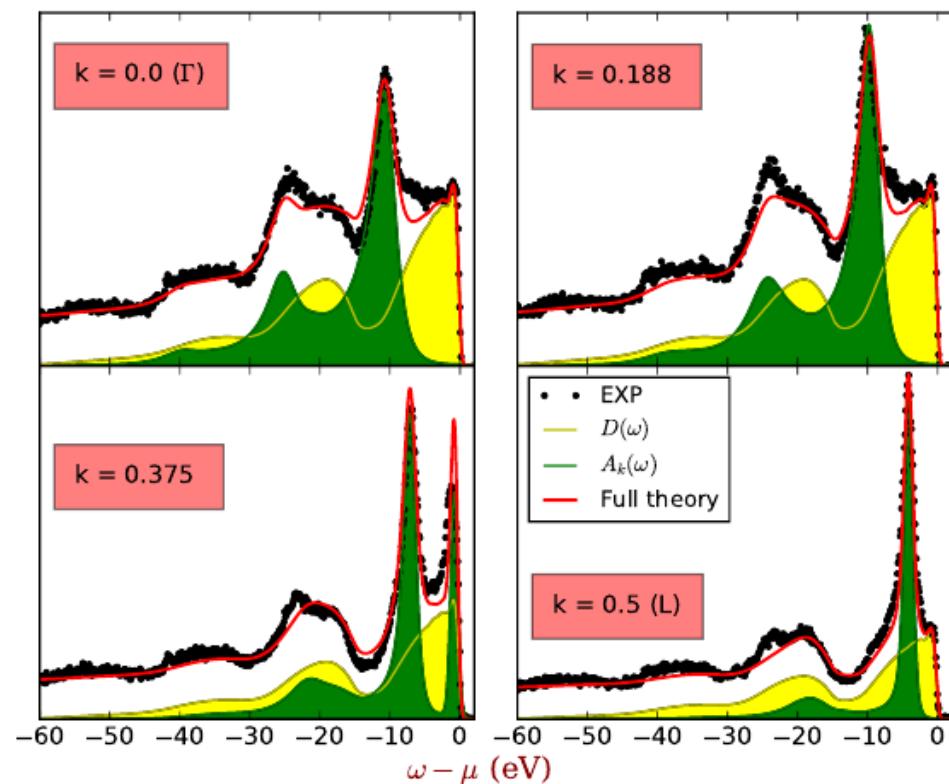
11/12/18

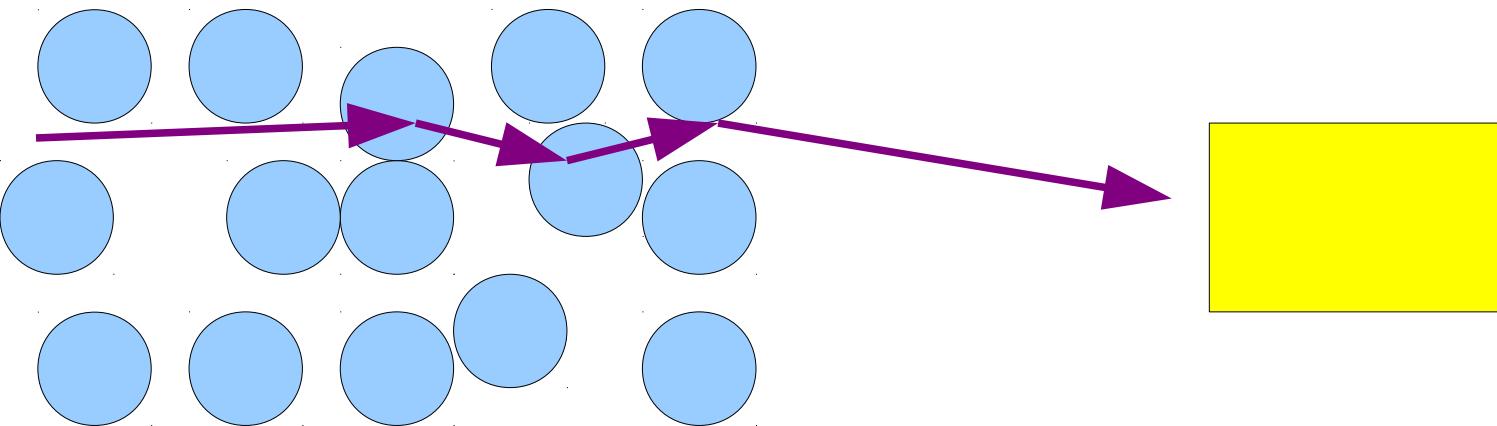




Zhou, Reining, Nicolaou, Bendoun  
Sirotti, Gatti, 2018.

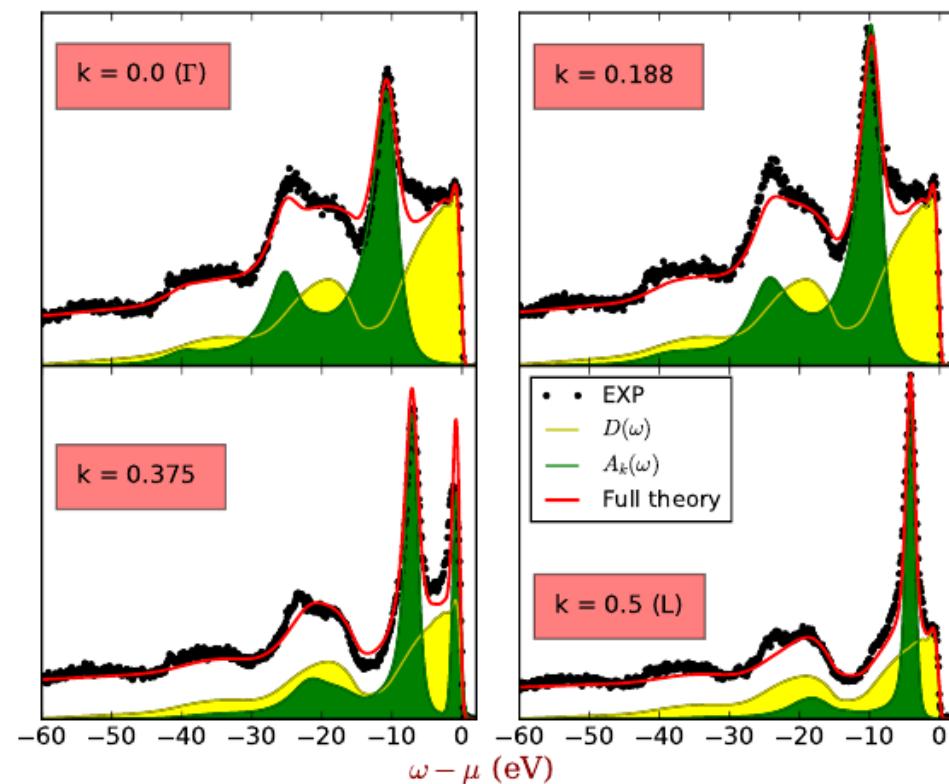
OV,

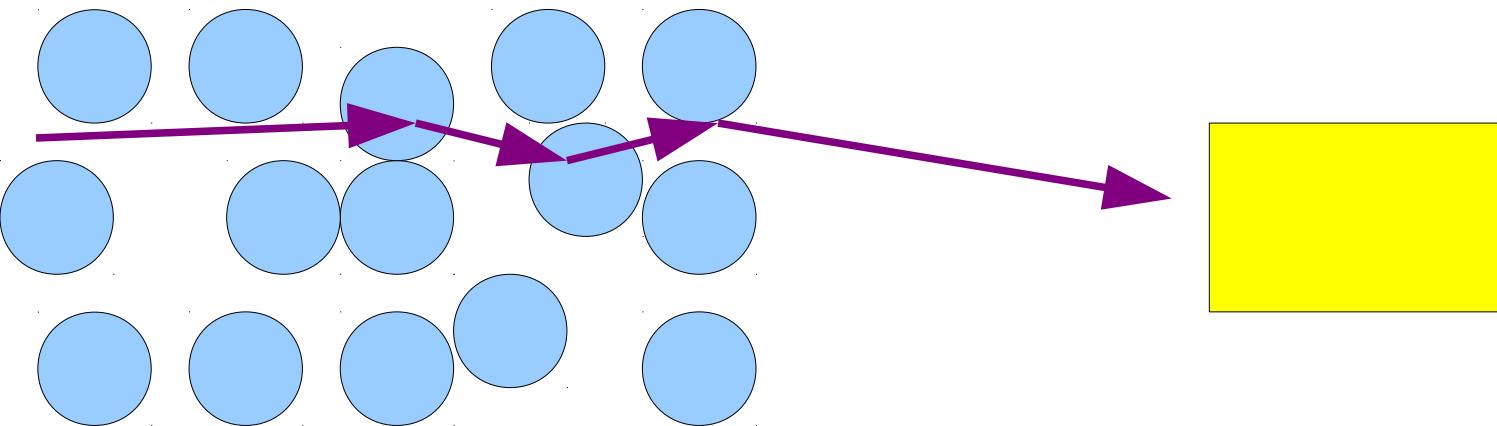




Zhou, Reining, Nicolaou, Bendoun  
Sirotti, Gatti, 2018.

DV,





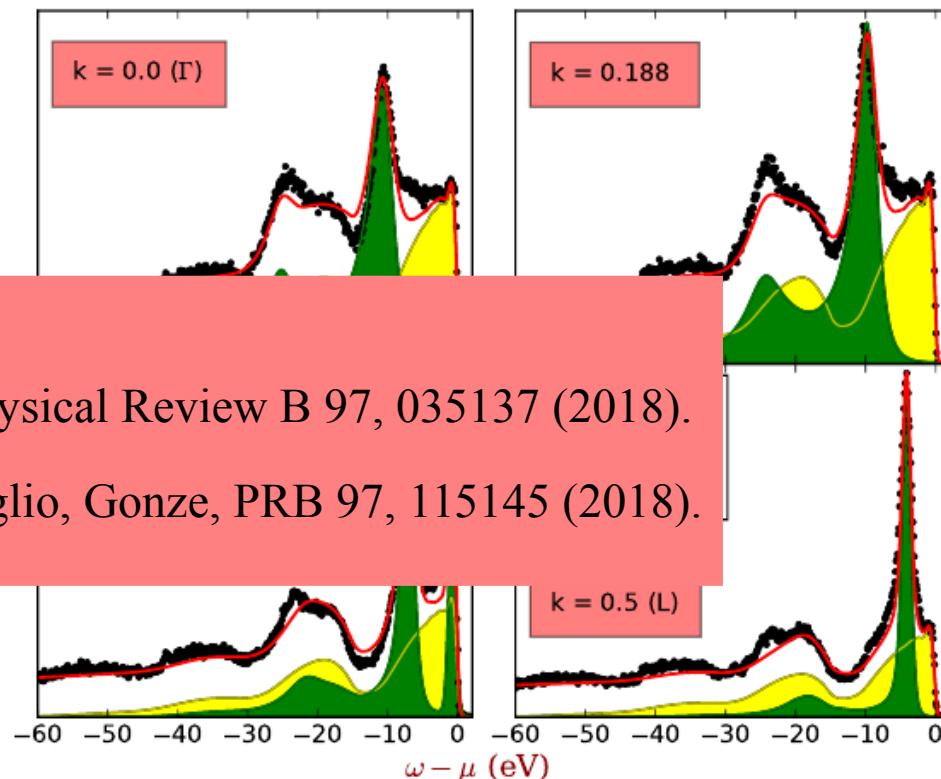
Zhou, Reining, Nicolaou, Bendoun  
Sirotti, Gatti, *arXiv*.....

ov,

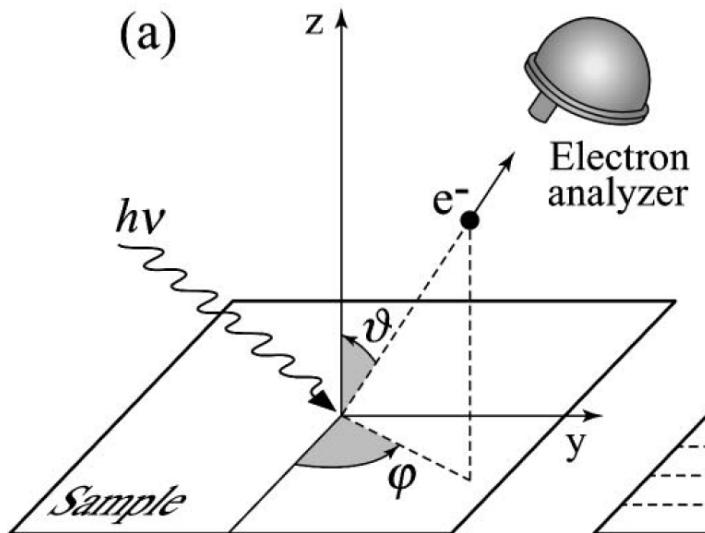
See also:

Zhou, Gatti, Kas, Rehr, Reining, Physical Review B 97, 035137 (2018).

Nery, Allen, Antonius, Reining, Miglio, Gonze, PRB 97, 115145 (2018).



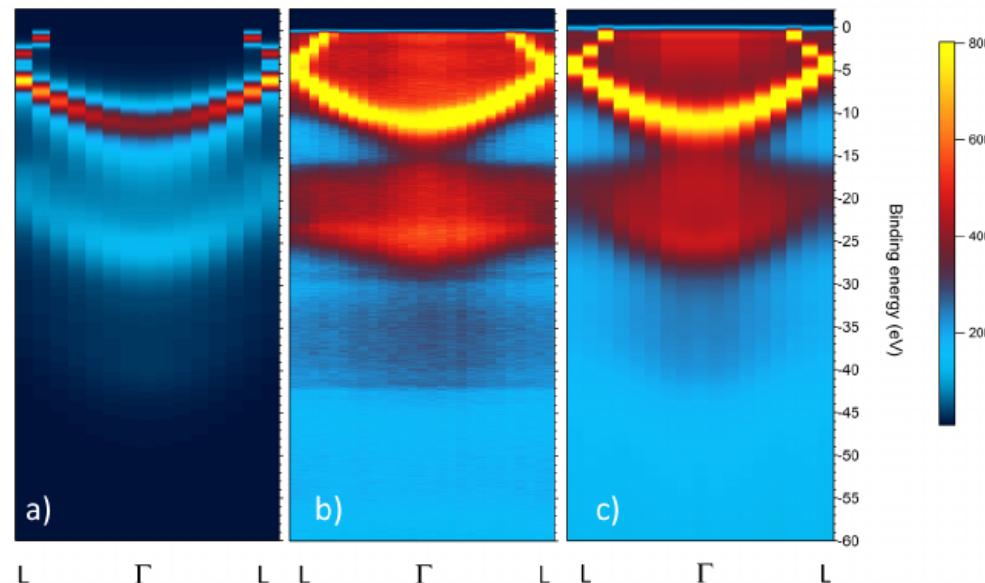
(a)



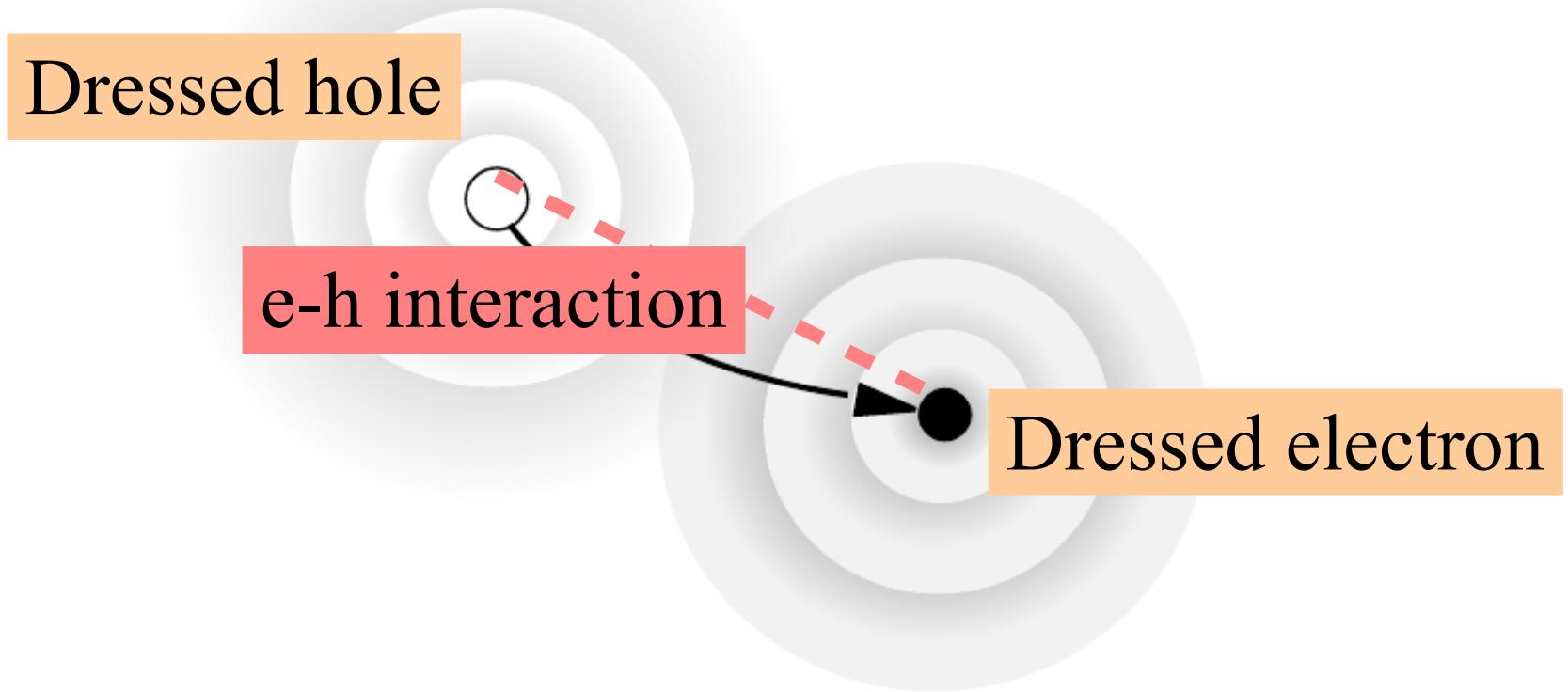
ARPES bulk aluminum

Exp.: Swiss Light Source

Zhou, Reining, Nicolaou, Bendounan, Ruotsalainen, Vanzini, Kas, Rehr, Muntwiler, Strocov, Sirotti, Gatti, 2018



→ Electron-hole correlation



e-h problem: Bethe-Salpeter (Dyson) equation  
Or  
Cumulant ansatz

→ The framework

→ Recycling I: → Cumulants

- \* *satellites in the one-body spectral function*
- \* *satellites in the two-body spectral function*

→ Recycling II: → Connector Theory

- \* *the dynamic structure factor*
- \* *the one-body spectral function*

→ Conclusions and outlook

## → Density response in TDDFT and BSE

1. Good descriptor: density  $n(r)$  → DFT

So, first we have to calculate the density

2. Auxiliary system → KS-DFT

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

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

## → Why are we here?

1. Good descriptor: density  $n(r)$  → DFT

So, first we have to calculate the density

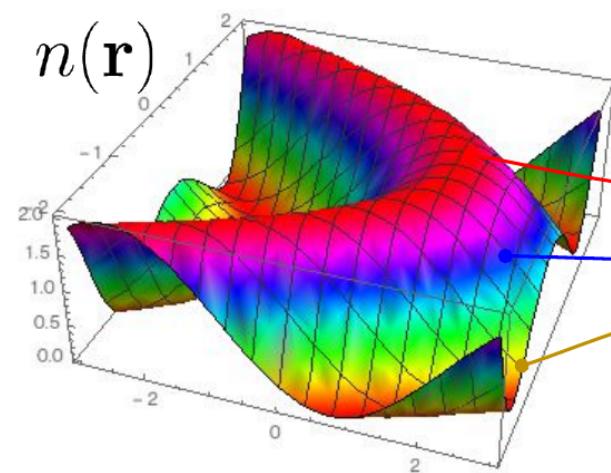
2. Auxiliary system → KS-DFT

So, first we have to calculate the xc potential

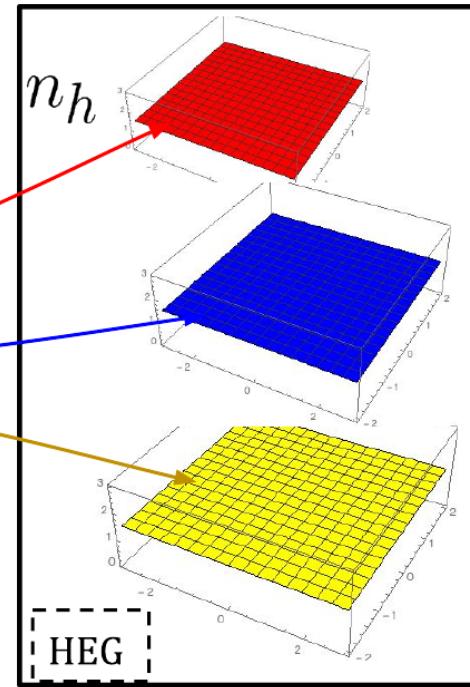
3. Model system → LDA

$$v_{\text{xc}}([n], r) \approx v_{\text{xc}}^{\text{HEG}}(n_r^h)$$

$$n_r^h = n(r)$$



$$\text{LDA}$$
$$n_h = n(\mathbf{r})$$



Used empirically in DFT-LDA!

## → Why are we here?

1. Good descriptor: density  $n(r)$  → DFT

So, first we have to calculate the density

2. Auxiliary system → KS-DFT

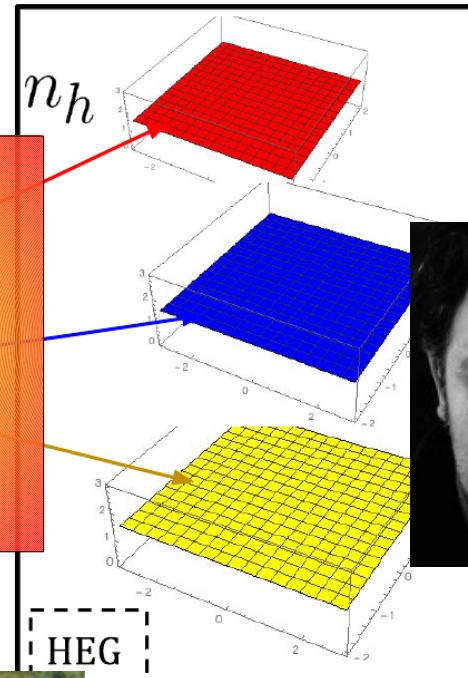
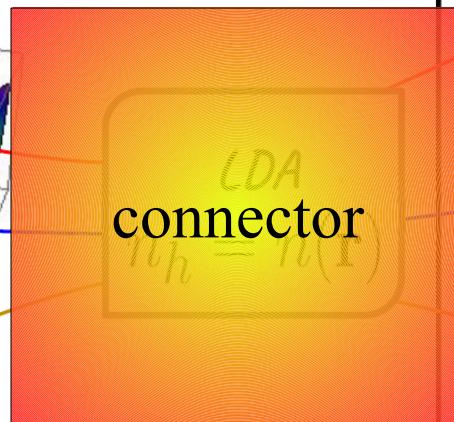
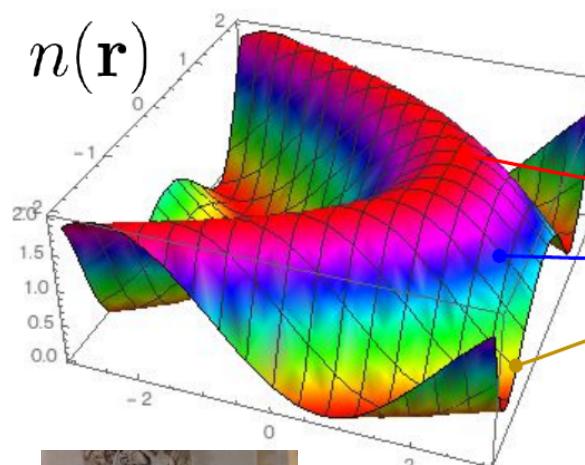
So, first we have to calculate the xc potential

3. Model system → LDA

$$v_{\text{xc}}([n], r) \approx v_{\text{xc}}^{\text{HEG}}(n_r^h) \quad v_{\text{xc}}([n], r) = v_{\text{xc}}^{\text{HEG}}(n_r^h)$$

$$n_r^h = n(r)$$

$$n_r^h \approx n(r)$$



Panholzer, Gatti, Reining, PRL 120, 166402 (2018); Vanzini, Reining, Gatti, EJPB91, 192 (2018) and arXiv:1708.02450; Vanzini, Aouina, Panholzer, Gatti, Reining, arXiv (2018)

# Why is this good?

LDA: Do an advanced (QMC) calculation in the HEGs

- but do it only **once and forever, and for everyone!**

D. M. Ceperley and B. J. Alder  
Phys. Rev. Lett. 45, 566 (1980)

# Why is this good?

1. General: do involved calculations in the model,  
once and forever, for everyone

# Why is this good?

1. General: do involved calculations in the model,  
once and forever, for everyone

Connector:  $V_{\text{aux}}^{\text{real}}([n], x) = V_{\text{aux}}^{\text{HEG}}(n^h, \tilde{x})$

$$n^h = [V_{\text{aux}}^{\text{HEG}}(\tilde{x})]^{-1}(V_{\text{aux}}^{\text{real}}([n], x))$$

$$n_{x\tilde{x}}^h[n] = [V_{\text{aux}}^{\text{HEG}}(\tilde{x})]^{-1}(V_{\text{aux}}^{\text{real}}([n], x))$$

# Why is this good?

1. General: do involved calculations in the model,

once and forever, for everyone

Connector:  $V_{\text{aux}}^{\text{real}}([n], x) = V_{\text{aux}}^{\text{HEG}}(n^h, \tilde{x})$

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# Why is this good?

1. General: do involved calculations in the model,

once and forever, for everyone

---

2. Connector: error canceling

$$n^h = [V_{\text{aux}}^{\text{HEG}}(\tilde{x})]^{-1}(V_{\text{aux}}^{\text{real}}([n], x))$$

$$n_{x\tilde{x}}^h[n] = [V_{\text{aux}}^{\text{HEG}}(\tilde{x})]^{-1}(V_{\text{aux}}^{\text{real}}([n], x))$$

## → Connector Theory: Example

*Target:* Hartree potential of finite system. *Model:* jellium sphere.

$$v_H(\mathbf{r}, [n]) = \int d\mathbf{r}' \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \stackrel{!}{=} n^{hom} \int_R d\mathbf{r}' \frac{1}{|\mathbf{r} - \mathbf{r}'|}$$

$$n^{hom}(\mathbf{r}, [n]) = \int d\mathbf{r}' \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \left/ \int_R d\mathbf{r}' \frac{1}{|\mathbf{r} - \mathbf{r}'|} \right.$$

$$v_H(\mathbf{r}, [n]) = v_H^{model}(\mathbf{r}, n^{hom}(\mathbf{r}))$$

Now approximate, e.g.  $\frac{1}{|\mathbf{r}-\mathbf{r}'|} \rightarrow c$

*In original expression:*

$$v_H(\mathbf{r}) \approx N*c$$

*In connector:*  $n^{hom}(\mathbf{r}, [n]) = \frac{1}{4\pi R^3/3} \int d\mathbf{r}' n(\mathbf{r}') = \bar{n}$  MDA

Correct long-range behaviour,  $c$  cancels!!!

$$v_H(\mathbf{r}) \approx \bar{n} \int_R d\mathbf{r}' \frac{1}{|\mathbf{r}-\mathbf{r}'|}$$

## → Connector Theory: Example

*Target:* Hartree potential of finite system. *Model:* jellium sphere.

$$v_H(\mathbf{r}, [n]) = \int d\mathbf{r}' \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \stackrel{!}{=} n^{hom} \int_R d\mathbf{r}' \frac{1}{|\mathbf{r} - \mathbf{r}'|}$$

**Errors due to approximations cancel in connector**

**Much better than same approx. directly on  $V^{\text{real}}$**

**Model system tabulated and used in simple way**

Now approximate, e.g.  $\frac{1}{|\mathbf{r} - \mathbf{r}'|} \sim \frac{1}{R}$

*In original expression:*

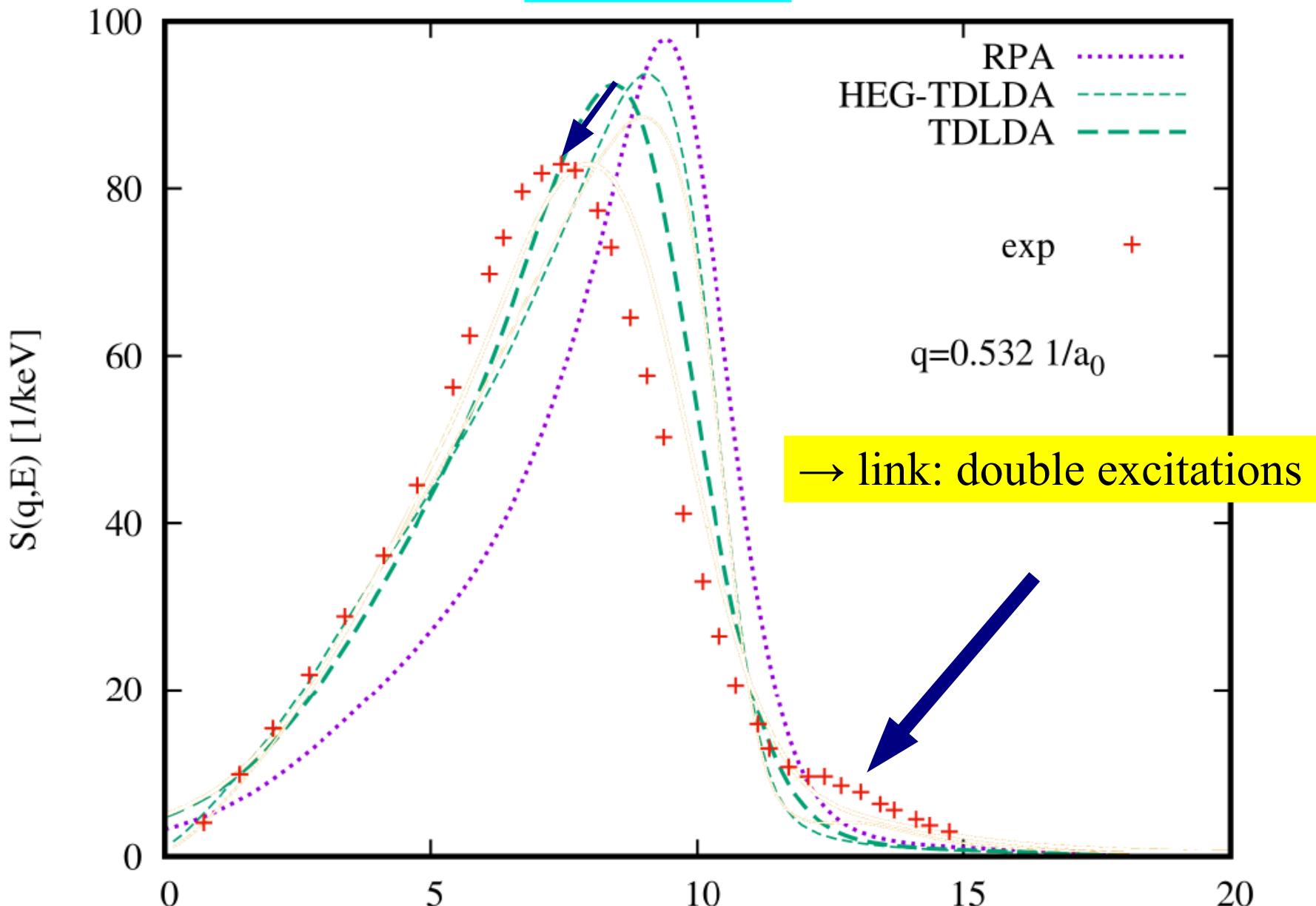
$$v_H(\mathbf{r}) \approx N/c$$

*In connector:*  $n^{hom}(\mathbf{r}, [n]) = \frac{1}{4\pi R^3/3} \int d\mathbf{r}' n(\mathbf{r}') = \bar{n}$

Correct long-range behaviour,  $c$  cancels!!!

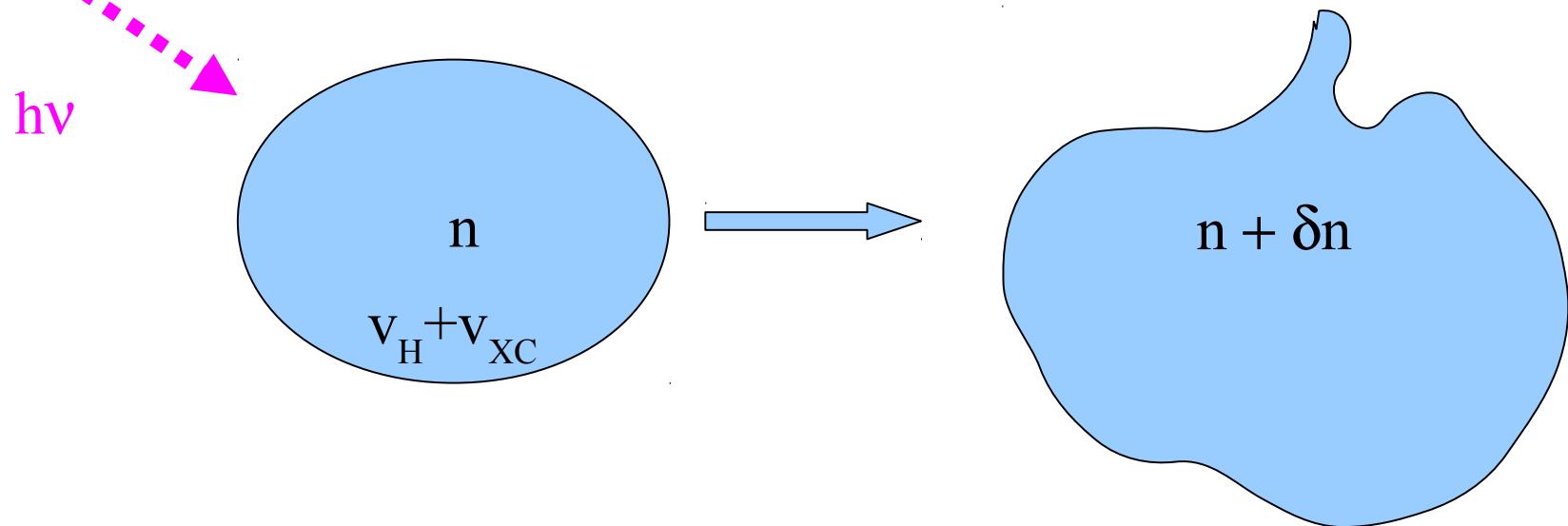
$$v_H(\mathbf{r}) \approx \bar{n} \int_R d\mathbf{r}' \frac{1}{|\mathbf{r} - \mathbf{r}'|}$$

# IXS-Sodium



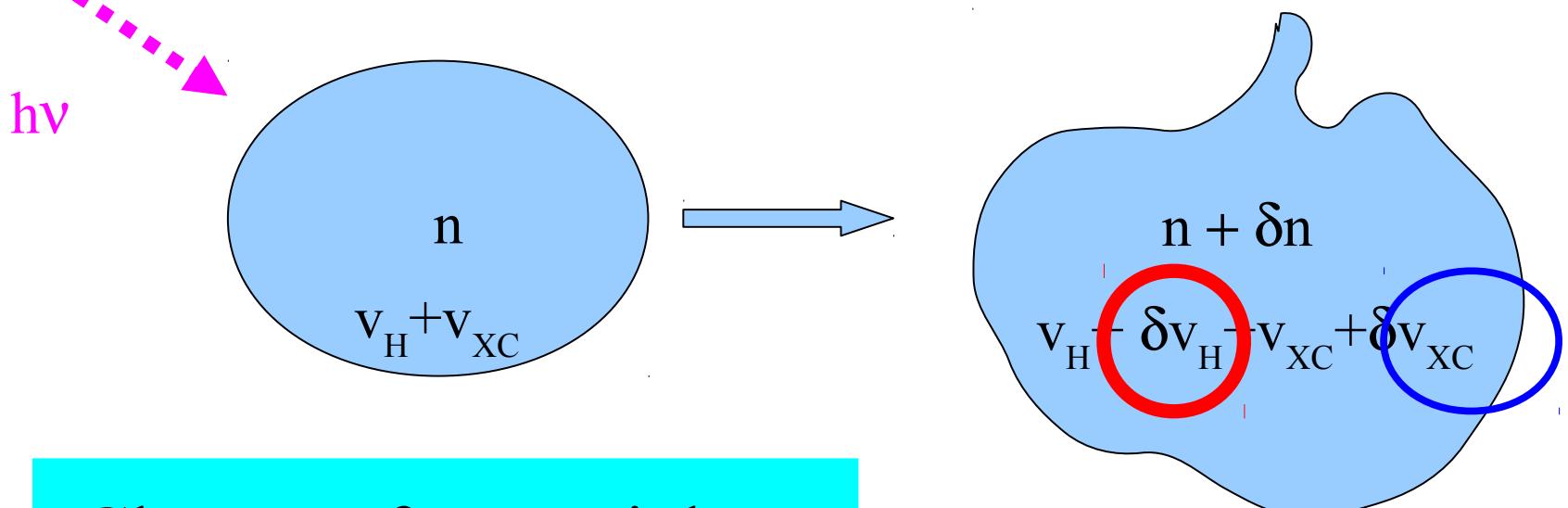
## Making it time-dependent:

(TD)DFT point of view: moving density



Excitation ?

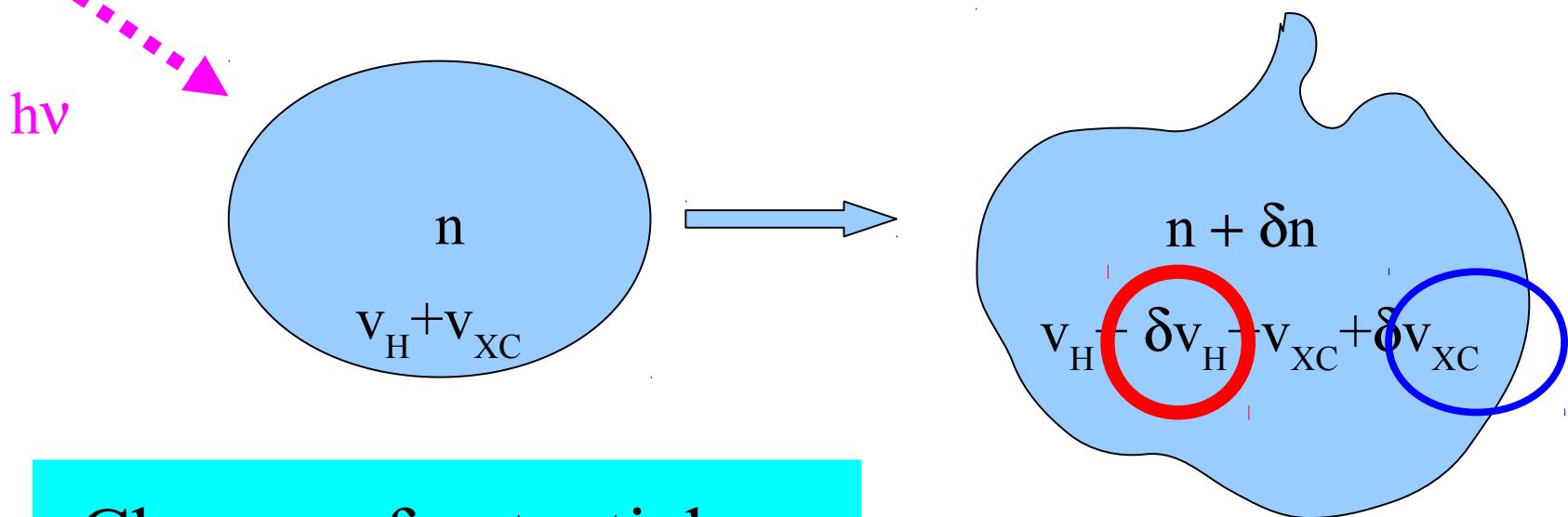
→ Induced potentials



Change of potentials

Excitation ?

→ Induced potentials



Change of potentials

RPA

ALDA, ....

Approximations

# Example : → the dynamic structure factor

$$S(q,\omega) \sim \text{Im} [\chi(q,\omega)]$$

In TDDFT,

$$\chi(q,\omega) = \chi_0(q,\omega) + \chi_{\perp}(q,\omega) \{v(q) + f_{xc}(q,\omega)\} \chi(q,\omega)$$

Auxiliary interaction

(Matrices in  $G, G'$ )

→ As a model system, we stay with the HEG

$v_{xc}$  in the HEG from QMC (Ceperley and Alder)

But  $f_{xc}$  ?

**Martin Panholzer** following

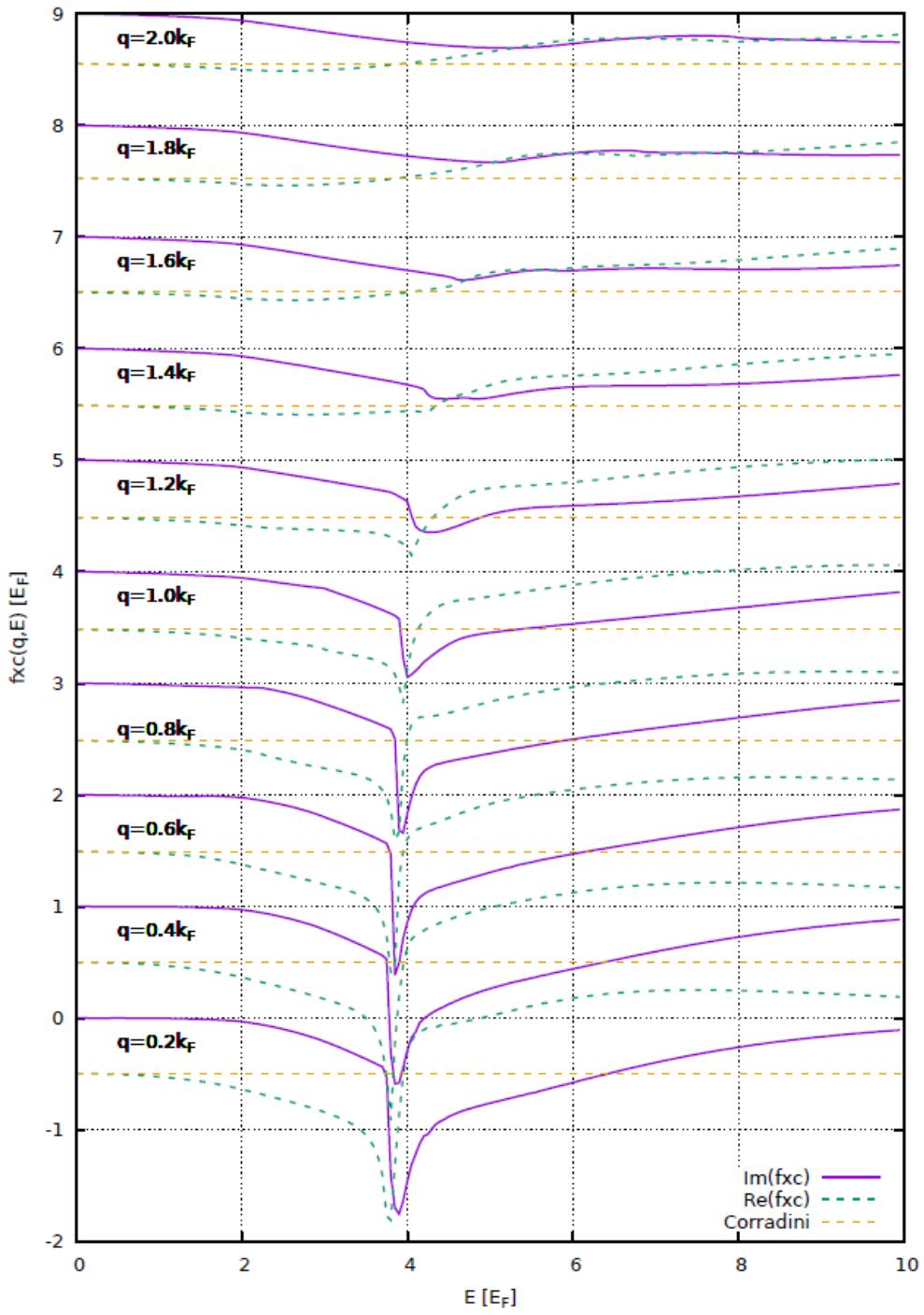
H. M. Boehm, R. Holler, E. Krotscheck, and M. Panholzer,  
Phys. Rev. B 82, 224505 (2010)

→ Calculate  $\chi$  in the HEG:

- action with Jastrow wavefunction
- linear response
- selected number of excitations
- $S(q)$  from QMC

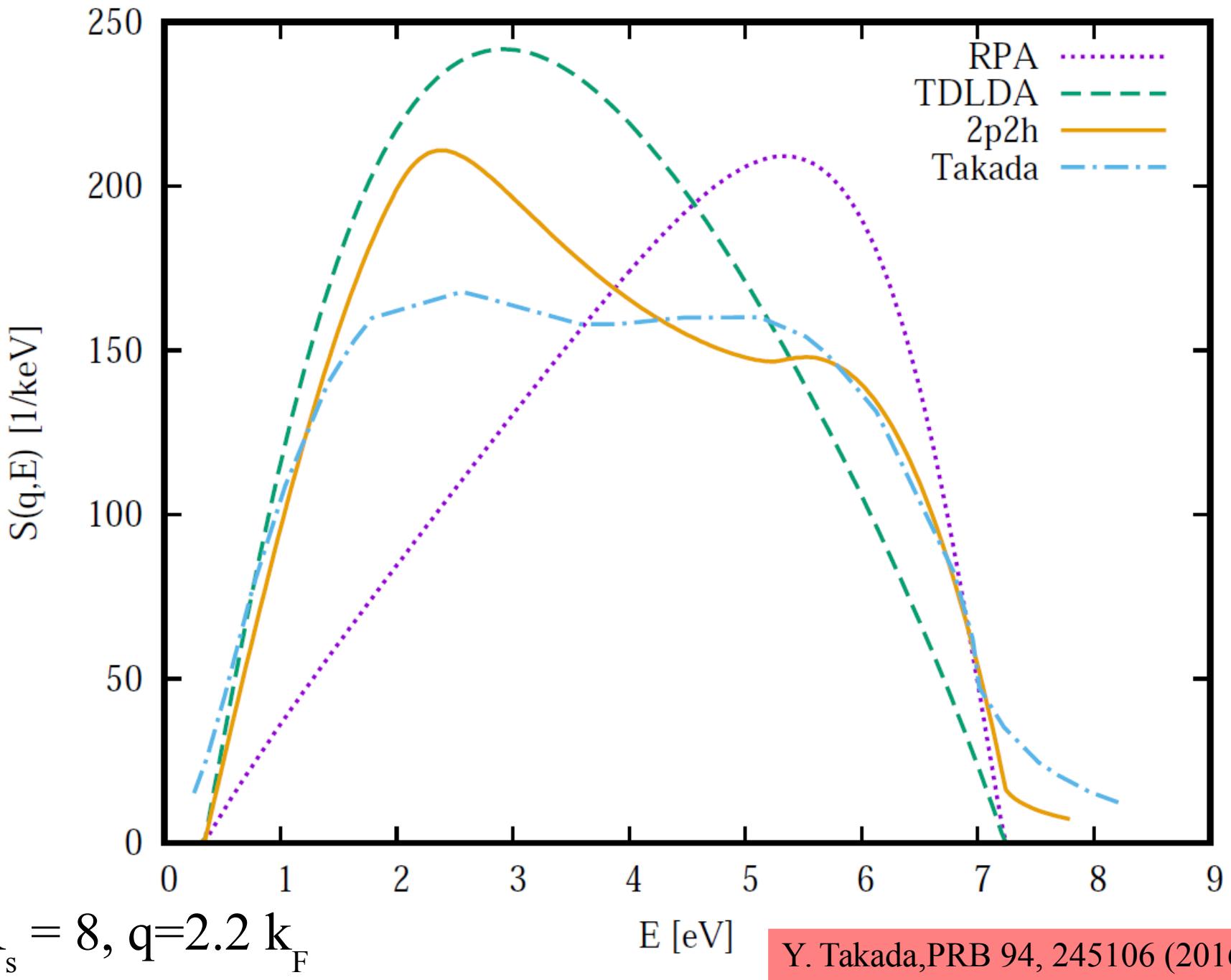
→ Calculate  $f_{xc}$  in the HEG by inverting  $\chi = \chi_0 + \chi_{\perp} [v + f_{xc}] \chi$

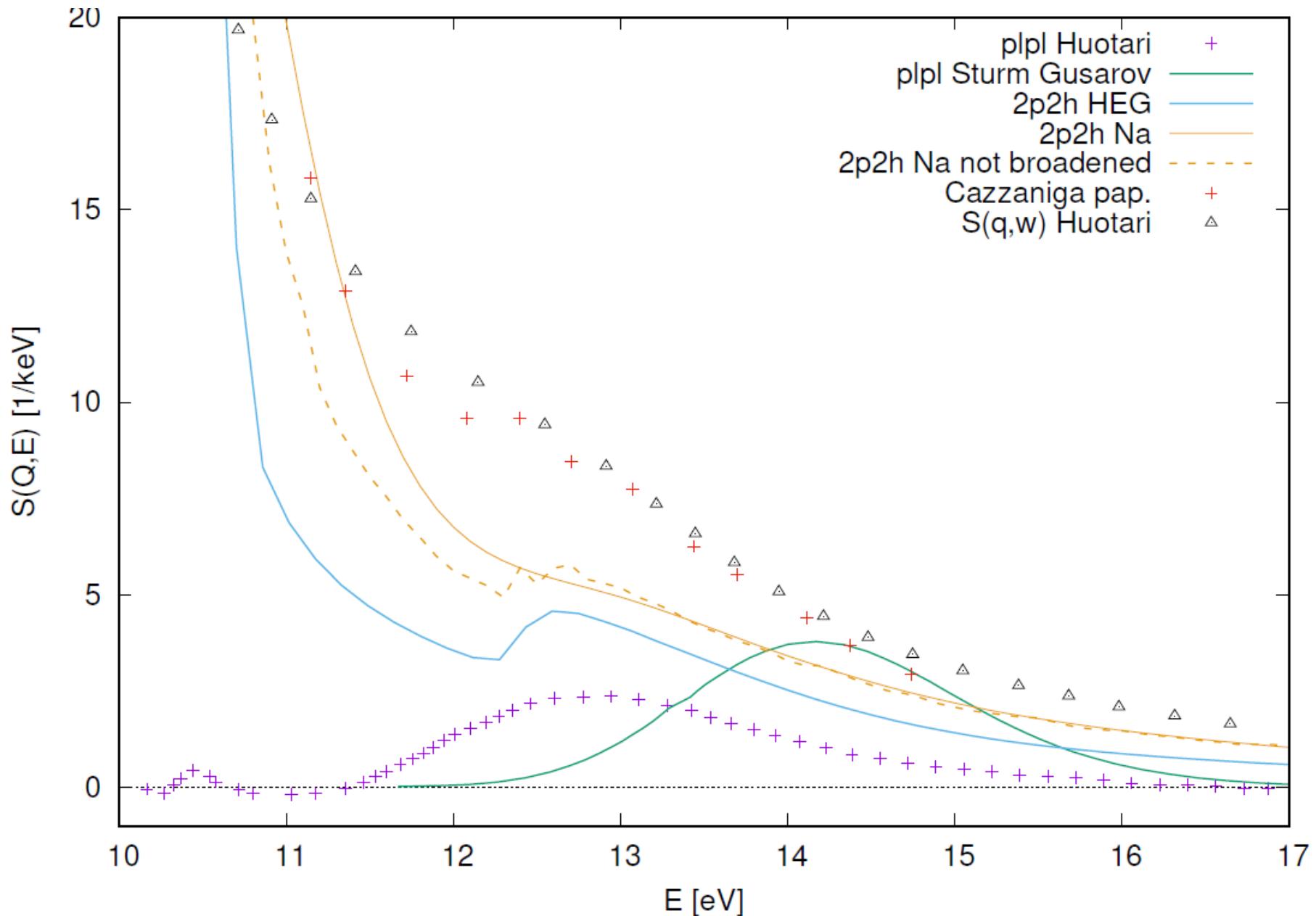
# HEG $f_{xc}$



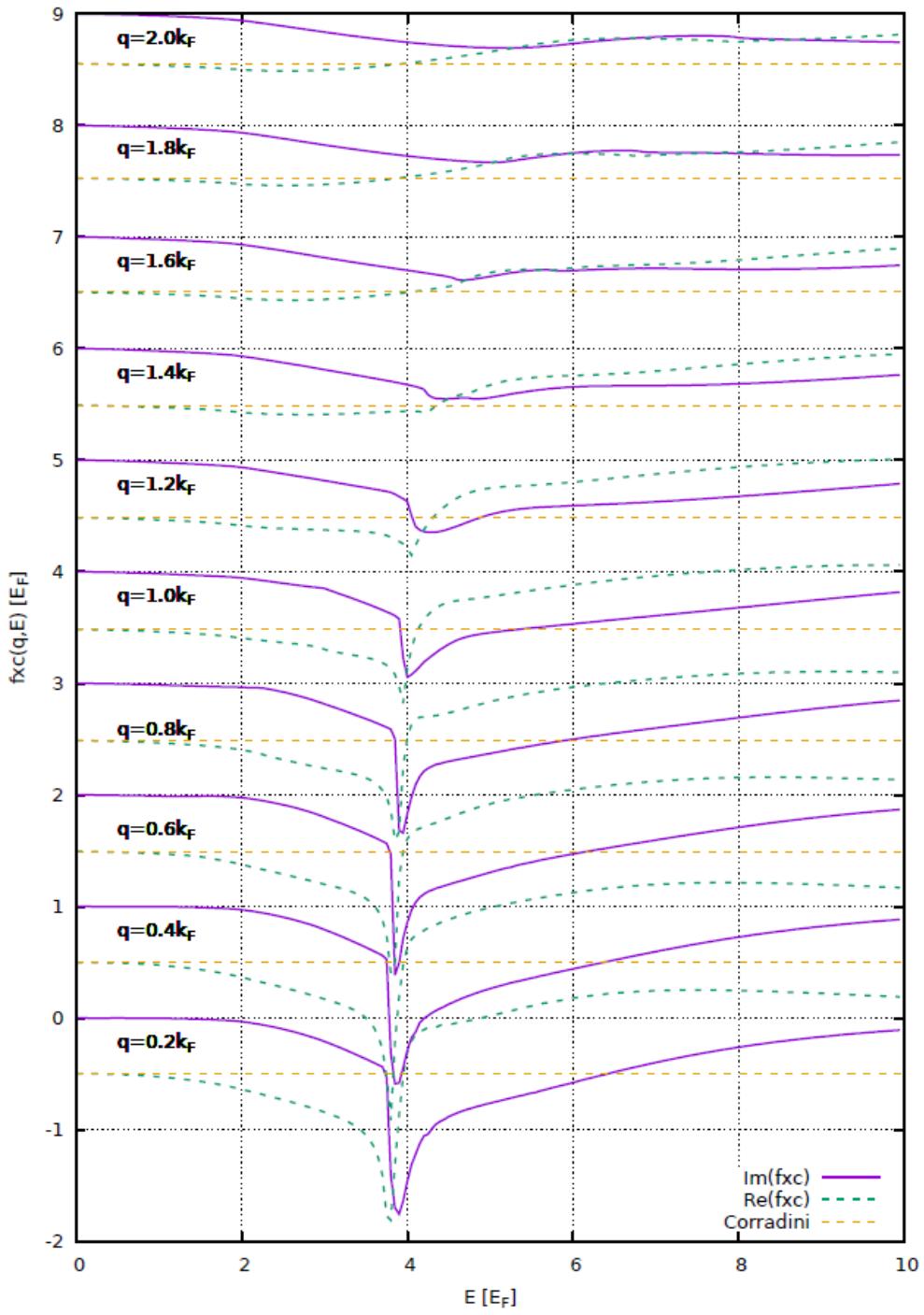
Static: M. Corradini, R. Del Sole,  
G. Onida, and M. Palummo,  
Phys. Rev. B 57, 14569 (1998).

Dynamic: Martin Panholzer et al.





# HEG $f_{xc}$

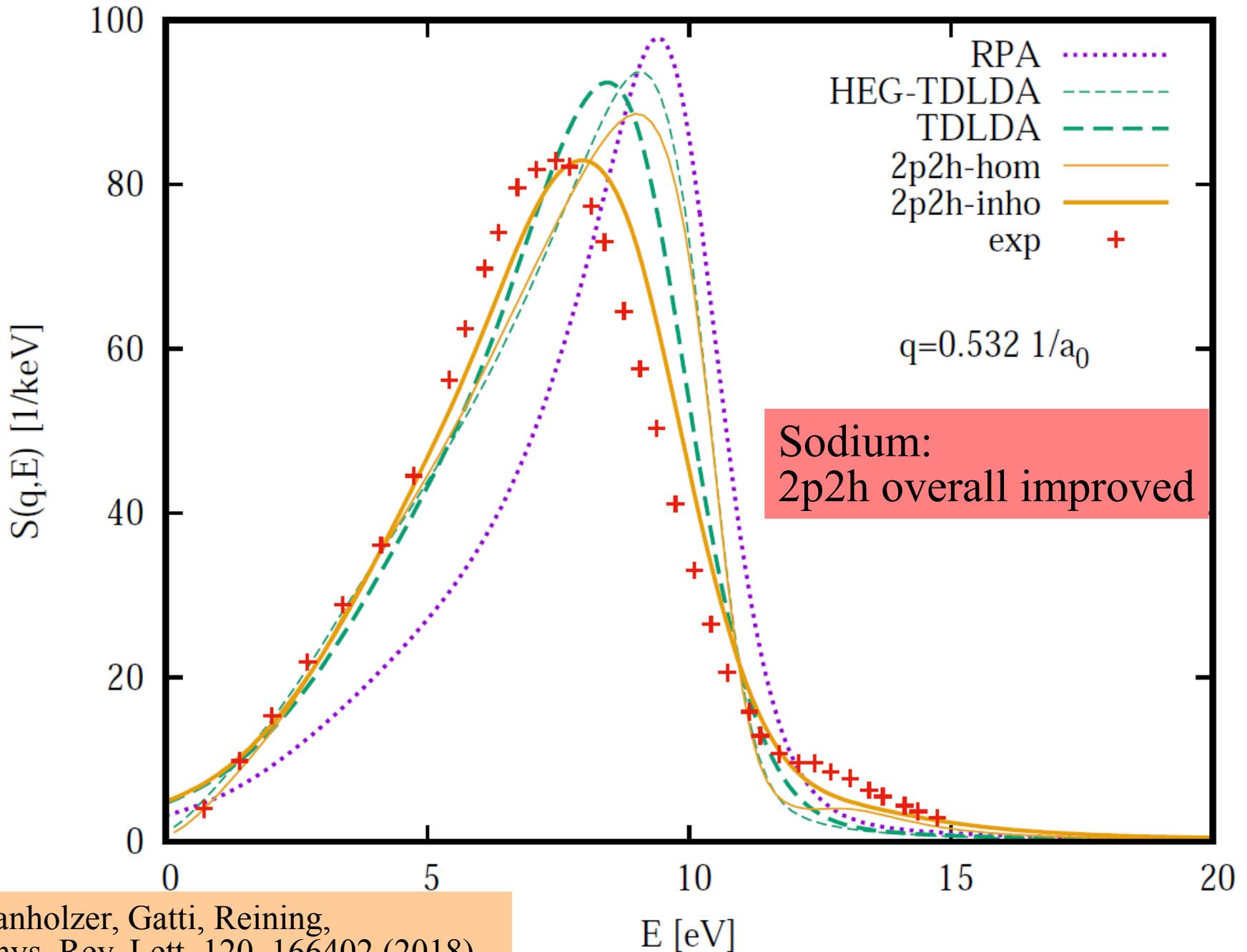


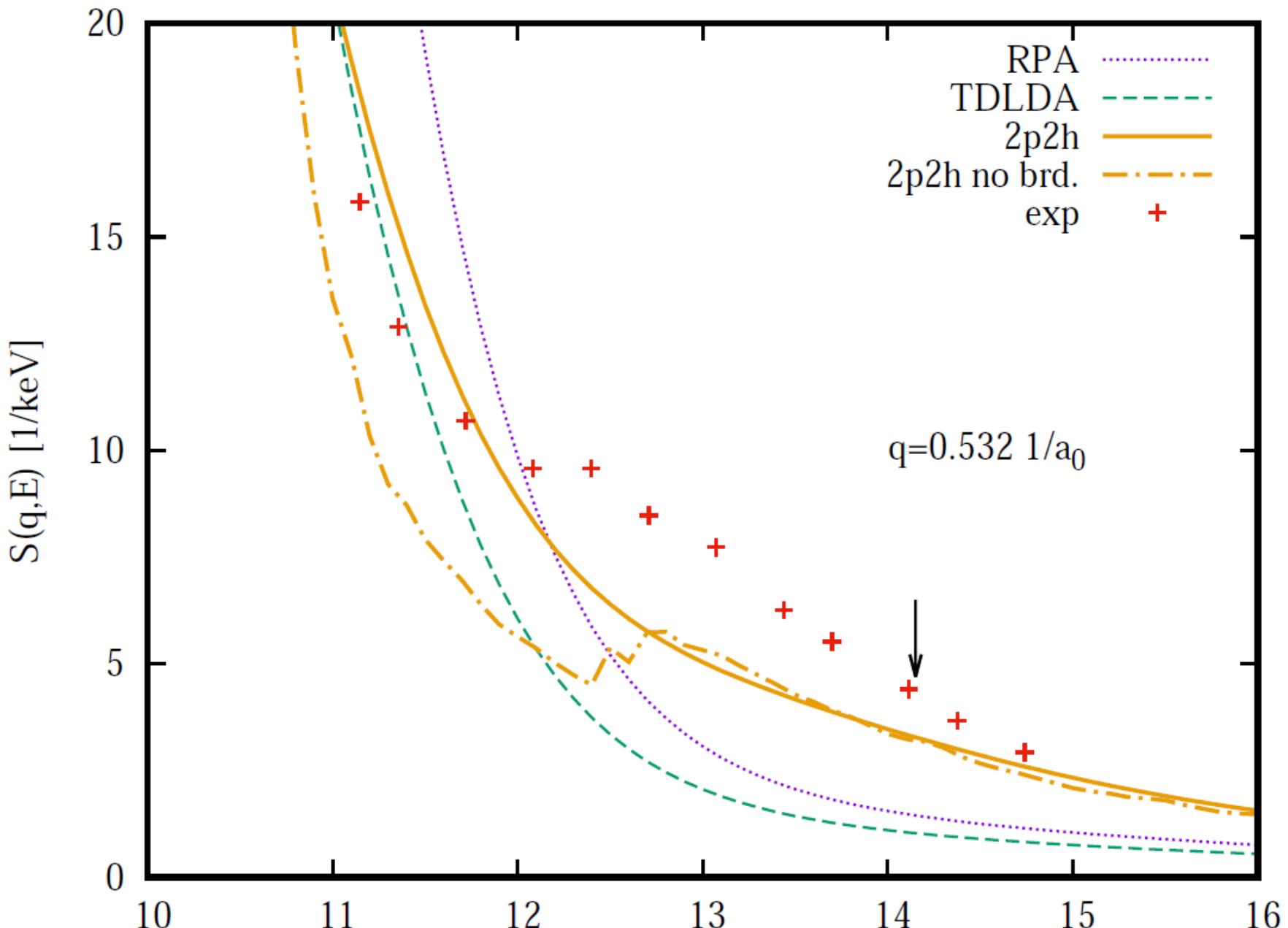
Static: M. Corradini, R. Del Sole,  
G. Onida, and M. Palummo,  
Phys. Rev. B 57, 14569 (1998).

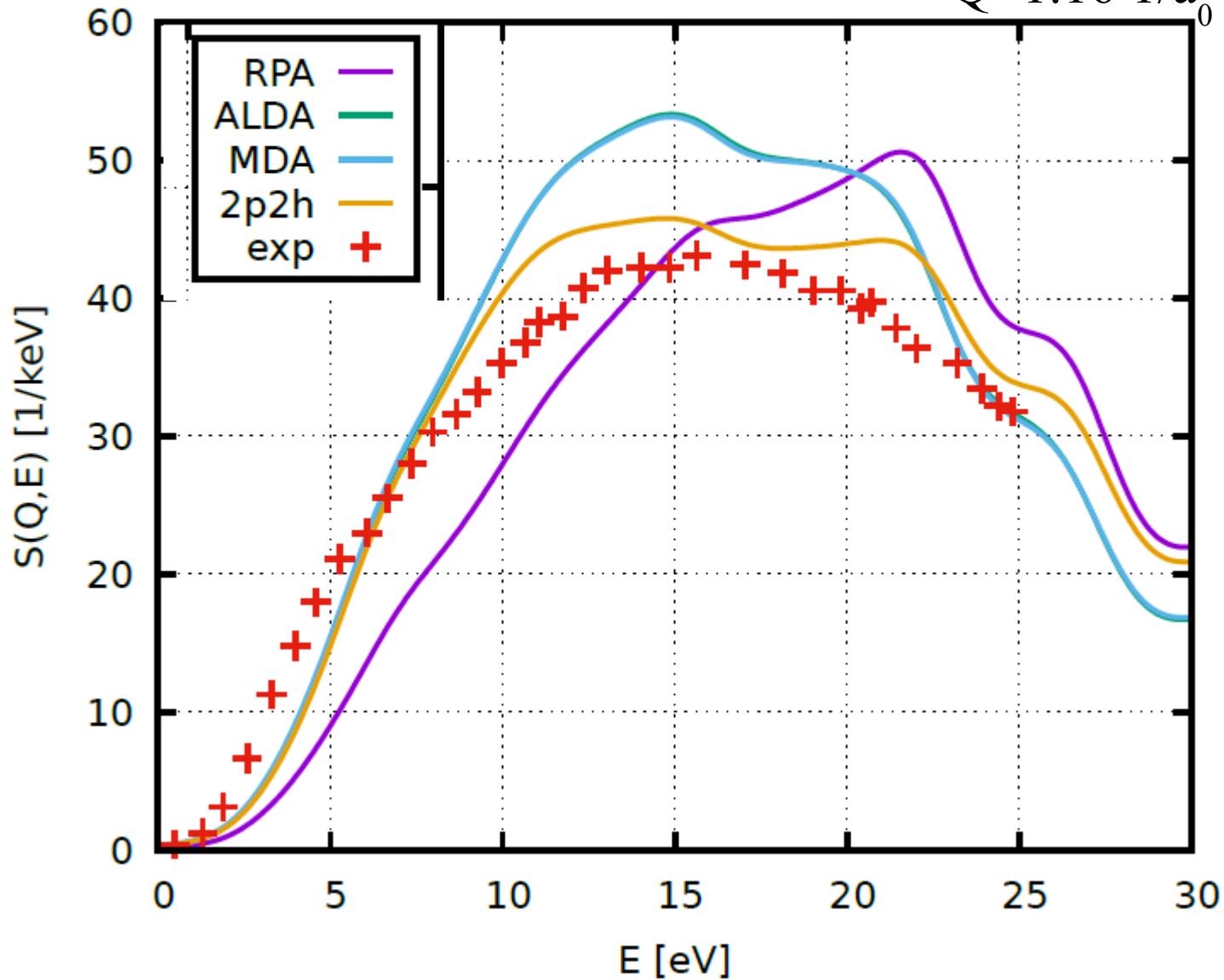
Dynamic: Martin Panholzer et al.

Connector for  $f_{xc}(r,t;r',t')$ :  
“mean density approximation”

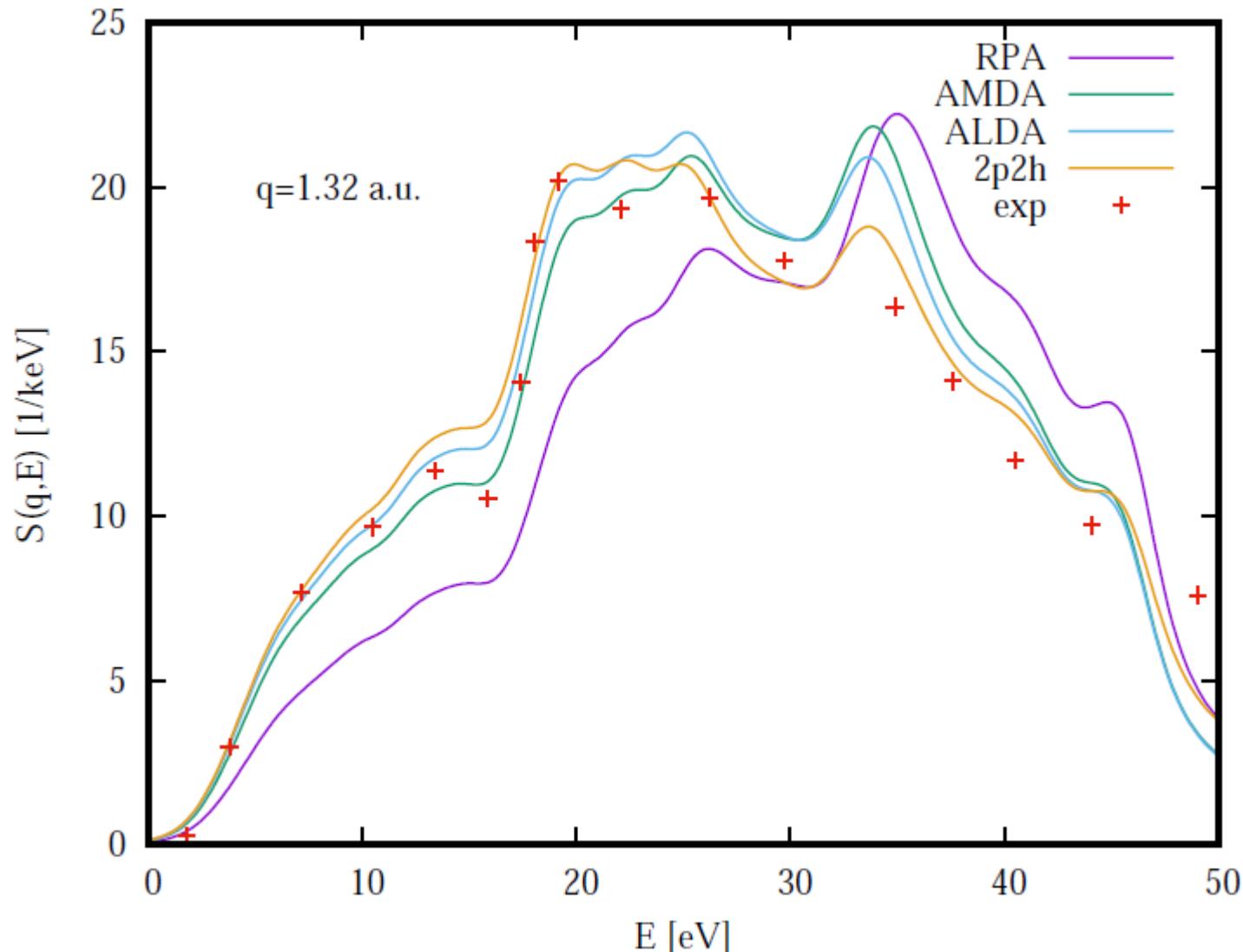
Panholzer, Gatti, Reining,  
Phys. Rev. Lett. 120, 166402 (2018)





$Q=1.16 \frac{1}{a_0}$ 

# Silicon



→ The framework

→ Recycling I: → Cumulants

- \* *satellites in the one-body spectral function*
- \* *satellites in the two-body spectral function*

→ Recycling II: → Connector Theory

- \* *the dynamic structure factor*
- \* *the one-body spectral function*

→ Conclusions and outlook

→ (One of ) the problem(s): memory effects

In time-dependent problems: often make adiabatic approximation

$$f_{\text{xc}}(\mathbf{r}, \mathbf{r}', t, t'; [n]) \rightarrow \delta(t - t') f_{\text{xc}}(\mathbf{r}, \mathbf{r}', \omega = 0; [n](t))$$

Consequences:

- \* e.g. after switching off perturbation,  $n(\mathbf{r}, t) \rightarrow v(\mathbf{r}, n(\mathbf{r}, t)) \rightarrow \omega_i(t)$
- \* wrong charge transfer
- \* cannot describe Rabi oscillations
- \* .....

Important work by:  
Maitra, Burke, Nest,...

→ (One of ) the problem(s): memory effects

$$f_{\text{xc}}(\mathbf{r}, \mathbf{r}', t - t'; [n]) \rightarrow f_{\text{xc}}(\mathbf{r}, \mathbf{r}', \omega; [n])$$

In equilibrium: memory →  $\omega$ -dependence

→ To understand how to include memory effects,  
we can study frequency-dependent interactions and potentials

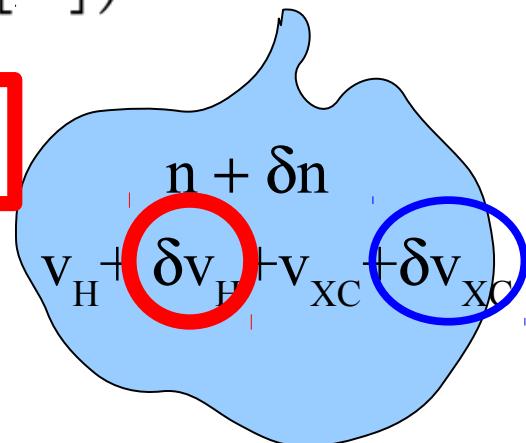
$$\frac{\delta v_H(\mathbf{r}, t; [n])}{\delta n(\mathbf{r}', t')} = \frac{\delta \int d\mathbf{x} v_c(\mathbf{r} - \mathbf{x}) n(\mathbf{x}, t)}{\delta n(\mathbf{r}', t')} = v_c(\mathbf{r} - \mathbf{r}')$$

$$\frac{\delta v_{xc}(\mathbf{r}, t; [n])}{\delta n(\mathbf{r}', t')} \equiv f_{xc}(\mathbf{r}, \mathbf{r}', t, t'; [n])$$

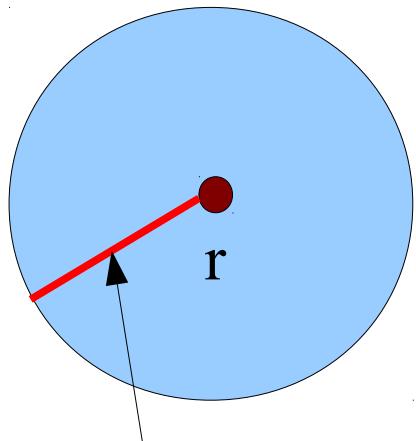
**Memory!**

$$f_{xc}(\mathbf{r}, \mathbf{r}', t - t'; [n]) \rightarrow f_{xc}(\mathbf{r}, \mathbf{r}', \omega; [n])$$

In equilibrium: memory  $\rightarrow \omega$  - dependence



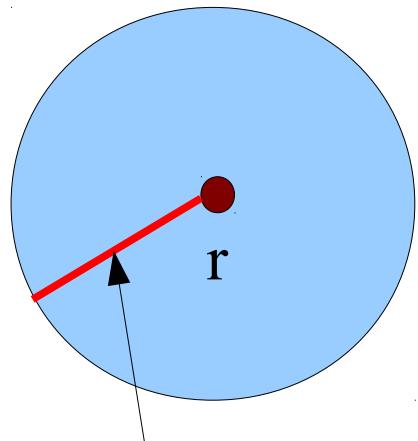
$$f_{xc}(r, r', \omega)$$



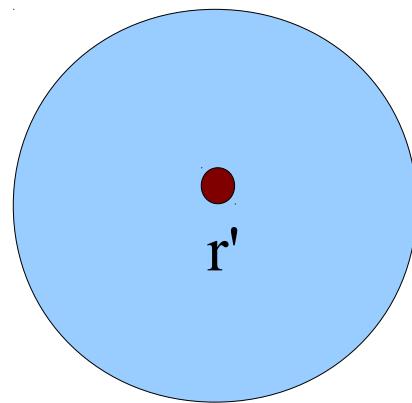
$$1.6 r_s$$

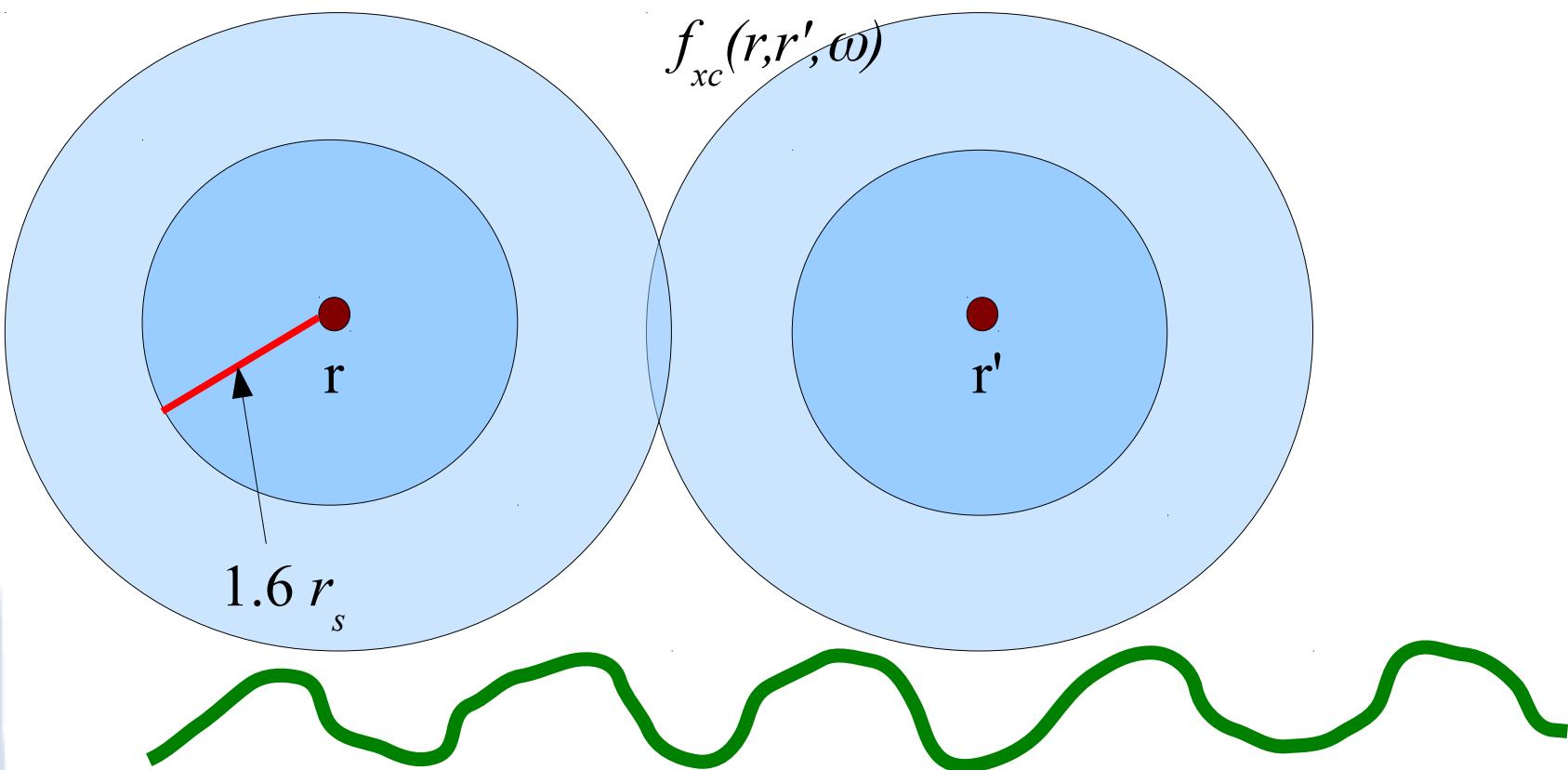
O. Gunnarsson, M. Jonson, and B. Lundqvist,  
Solid State Communications 24, 765 (1977);  
Phys. Rev. B 20, 3136 (1979).

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



$$1.6 r_s$$





Interatomic distances:     $\text{Na} = 1.75 r_s$      $\text{Si} = 2.2 r_s$

→ Mean Density Approximation

See also V. U. Nazarov, G. Vignale, and Y.-C. Chang,  
Phys. Rev. Lett. 102, 113001 (2009).

$$\Delta v^{xc}(\mathbf{r}, t)[n, \bar{n}] = \sum_{\mathbf{G}} \int_{1BZ} \frac{d^3 q}{(2\pi)^3} \int \frac{dw}{2\pi} e^{i(\mathbf{q} \cdot \mathbf{r} - wt)} e^{i\mathbf{G} \cdot \mathbf{r}} \delta n(\mathbf{q} + \mathbf{G}, w) f_{\mathbf{G}, \mathbf{G}}^{xc}(\mathbf{q}, w)[\bar{n}]$$

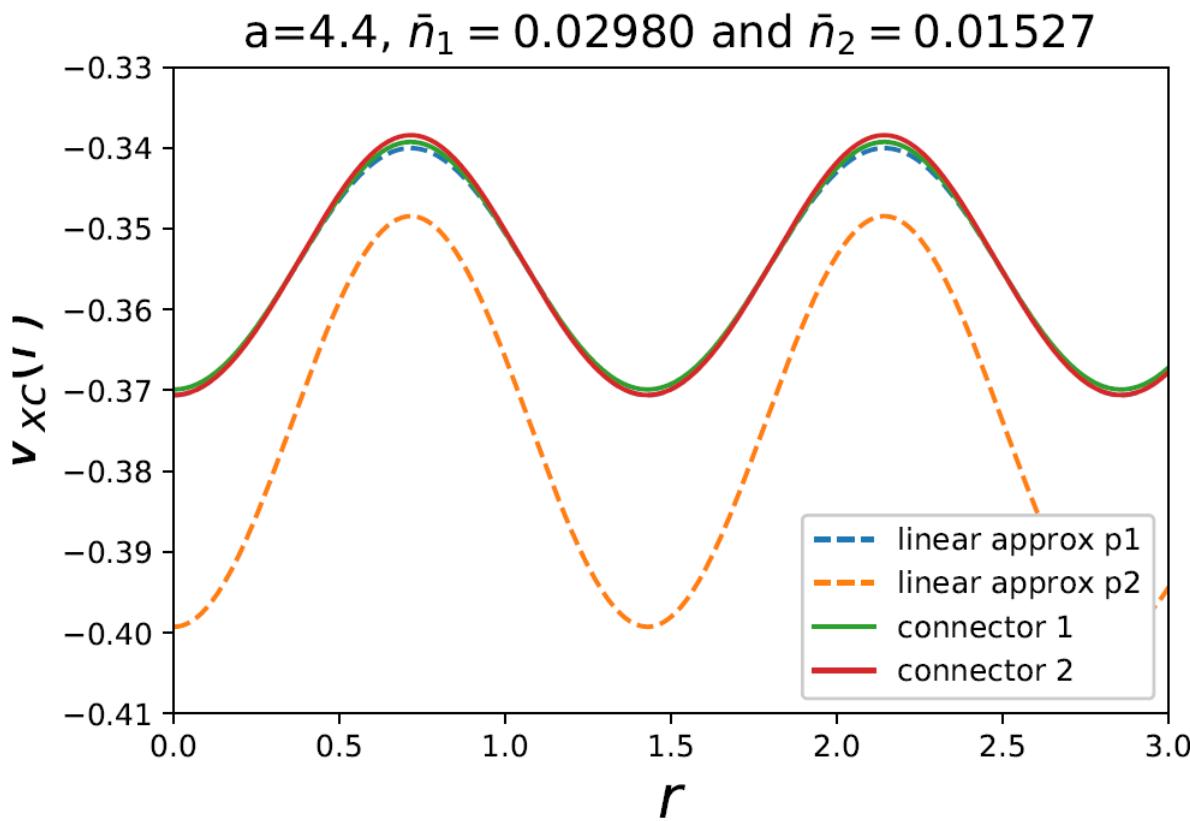
$$\Delta v^{xc}(\mathbf{r}, t)[n^h, \bar{n}^h] = \Delta n^h f_h^{xc}(\bar{n}^h)$$

$$\Delta v^{xc}(\mathbf{r}, t)[n, \bar{n}] = \Delta v^{xc}(\mathbf{r}, t)[n^h, \bar{n}^h]$$

$$n^h = \bar{n}^h + \sum_{\mathbf{G}} \int_{1BZ} \frac{d^3 q}{(2\pi)^3} \int \frac{dw}{2\pi} e^{i(\mathbf{q} \cdot \mathbf{r} - wt)} e^{i\mathbf{G} \cdot \mathbf{r}} \Delta n(\mathbf{q} + \mathbf{G}, w) \frac{f_{\mathbf{G}}^{xc}(\mathbf{q}, w)[\bar{n}]}{f_h^{xc}(\bar{n})}$$

$$n_{\mathbf{r}}^{con} = \frac{1}{f^{CODP}(\bar{n})} \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k.r}} n(\mathbf{k}) f^{xc}(\mathbf{k}, \bar{n})$$

$$\Delta n(\mathbf{r}) = B \cos(\mathbf{a.r}) + A$$



$$a=0.4, \bar{n}_1 = 0.00557092 \text{ and } \bar{n}_2 = 0.008846426$$

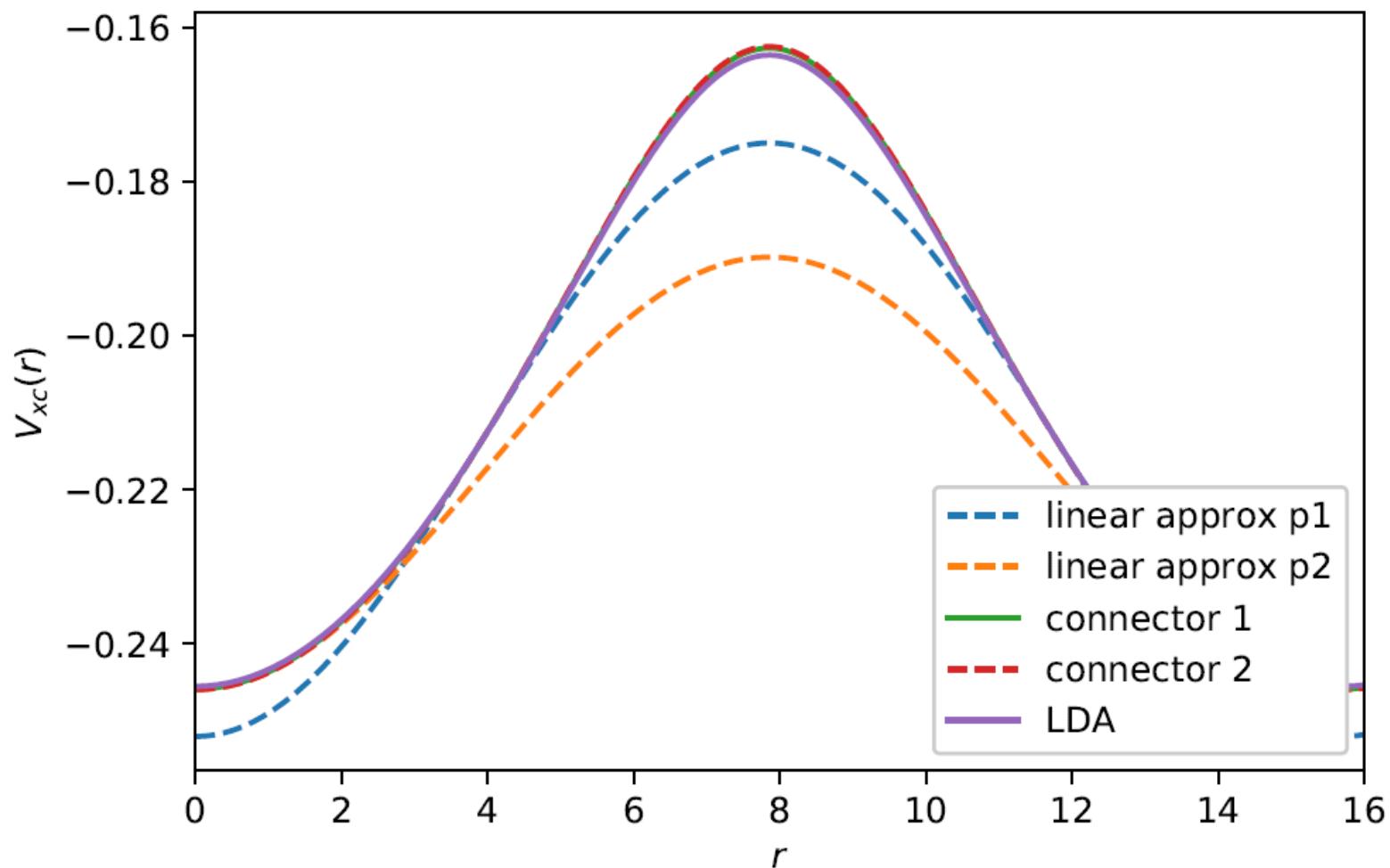
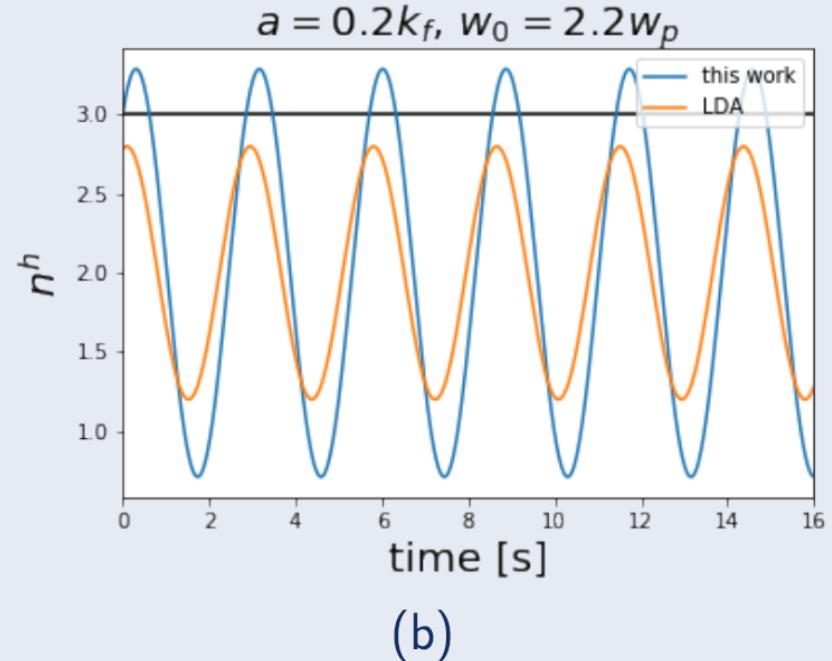
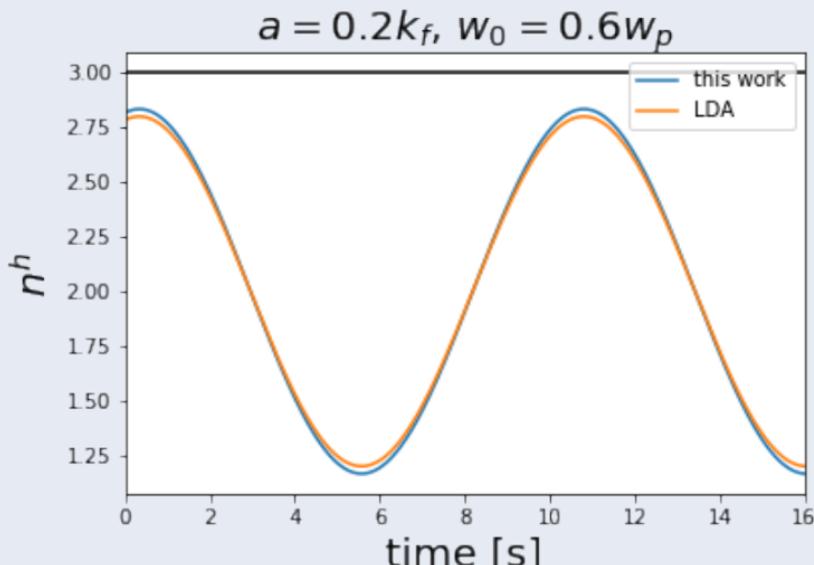
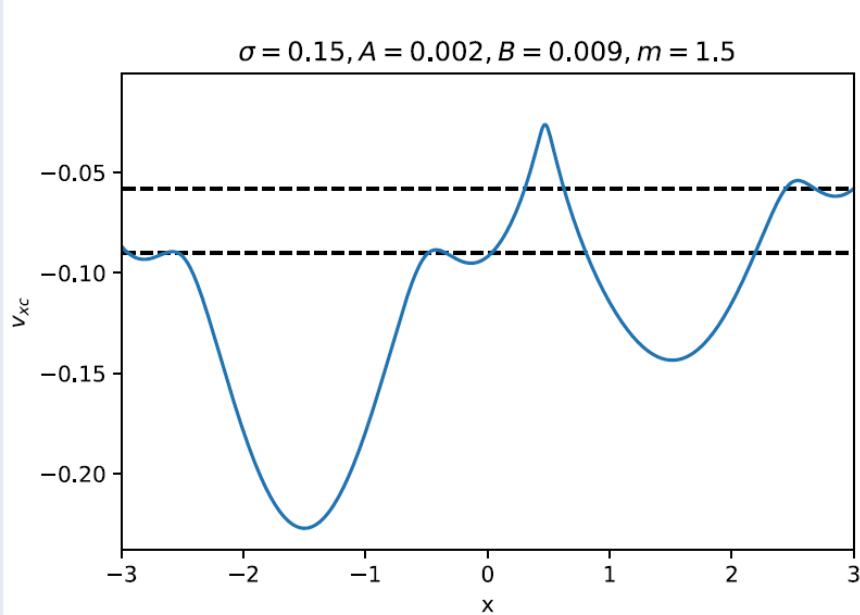


Figure 15: Two different starting points : the mean and the maximum of the density in the case of slowly varying density  $|a| = 0.4$

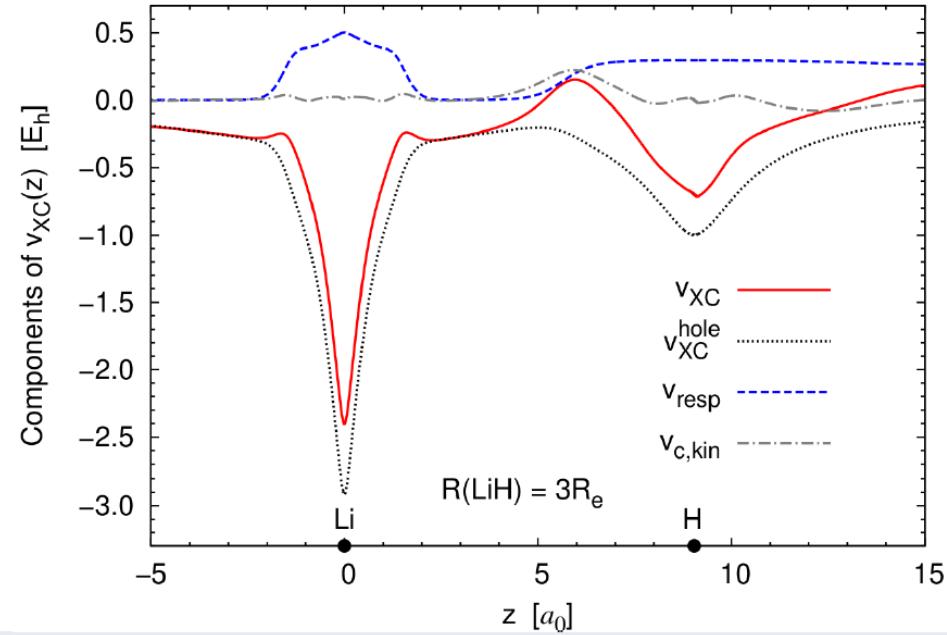
- Time dependent density:  $n(\mathbf{r}, t) = A \cos(\mathbf{a} \cdot \mathbf{r} - \omega t) + B$



- Gaussian density:  $n(\mathbf{r}) = Ae^{-\frac{1}{2\sigma}(\mathbf{r}-\mathbf{m})^2} + Be^{-\frac{1}{2\sigma}(\mathbf{r}+\mathbf{m})^2}$



(a) exchange correlation potential for two gaussian densities using connector strategy



(b) The exchange correlation potential of LiH taken from [4]

[4] S. V. Kohut et al.

*Phys. Chem. Chem. Phys.*, 18:20938, (2016).

## → Connector Theory: Example

*Target:* Hartree potential of finite system. *Model:* jellium sphere.

$$v_H(\mathbf{r}, [n]) = \int d\mathbf{r}' \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \stackrel{!}{=} n^{hom} \int_R d\mathbf{r}' \frac{1}{|\mathbf{r} - \mathbf{r}'|}$$

$$n^{hom}(\mathbf{r}, [n]) = \int d\mathbf{r}' \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \left/ \int_R d\mathbf{r}' \frac{1}{|\mathbf{r} - \mathbf{r}'|} \right.$$

$$v_H(\mathbf{r}, [n]) = v_H^{model}(\mathbf{r}, n^{hom}(\mathbf{r}))$$

Now approximate, e.g.  $\frac{1}{|\mathbf{r}-\mathbf{r}'|} \rightarrow c$

*In original expression:*

$$v_H(\mathbf{r}) \approx N*c$$

*In connector:*  $n^{hom}(\mathbf{r}, [n]) = \frac{1}{4\pi R^3/3} \int d\mathbf{r}' n(\mathbf{r}') = \bar{n}$  MDA

Correct long-range behaviour,  $c$  cancels!!!

$$v_H(\mathbf{r}) \approx \bar{n} \int_R d\mathbf{r}' \frac{1}{|\mathbf{r}-\mathbf{r}'|}$$

## → Connector Theory: Example

*Target:* Hartree potential of finite system. *Model:* jellium sphere.

$$v_H(\mathbf{r}, [n]) = \int d\mathbf{r}' \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \stackrel{!}{=} n^{hom} \int_R d\mathbf{r}' \frac{1}{|\mathbf{r} - \mathbf{r}'|}$$

**Errors due to approximations cancel in connector**

**Model system tabulated and used in simple way**

$$v_H(\mathbf{r}, [n]) = v_H^{model}(\mathbf{r}, n^{hom}(\mathbf{r}))$$

Now approximate, e.g.  $\frac{1}{|\mathbf{r}-\mathbf{r}'|} \rightarrow c$

*In original expression:*

$$v_H(\mathbf{r}) \approx N/c$$

*In connector:*  $n^{hom}(\mathbf{r}, [n]) = \frac{1}{4\pi R^3/3} \int d\mathbf{r}' n(\mathbf{r}') = \bar{n}$

Correct long-range behaviour,  $c$  cancels!!!

$$v_H(\mathbf{r}) \approx \bar{n} \int_R d\mathbf{r}' \frac{1}{|\mathbf{r}-\mathbf{r}'|}$$

# Example : → the dynamic structure factor

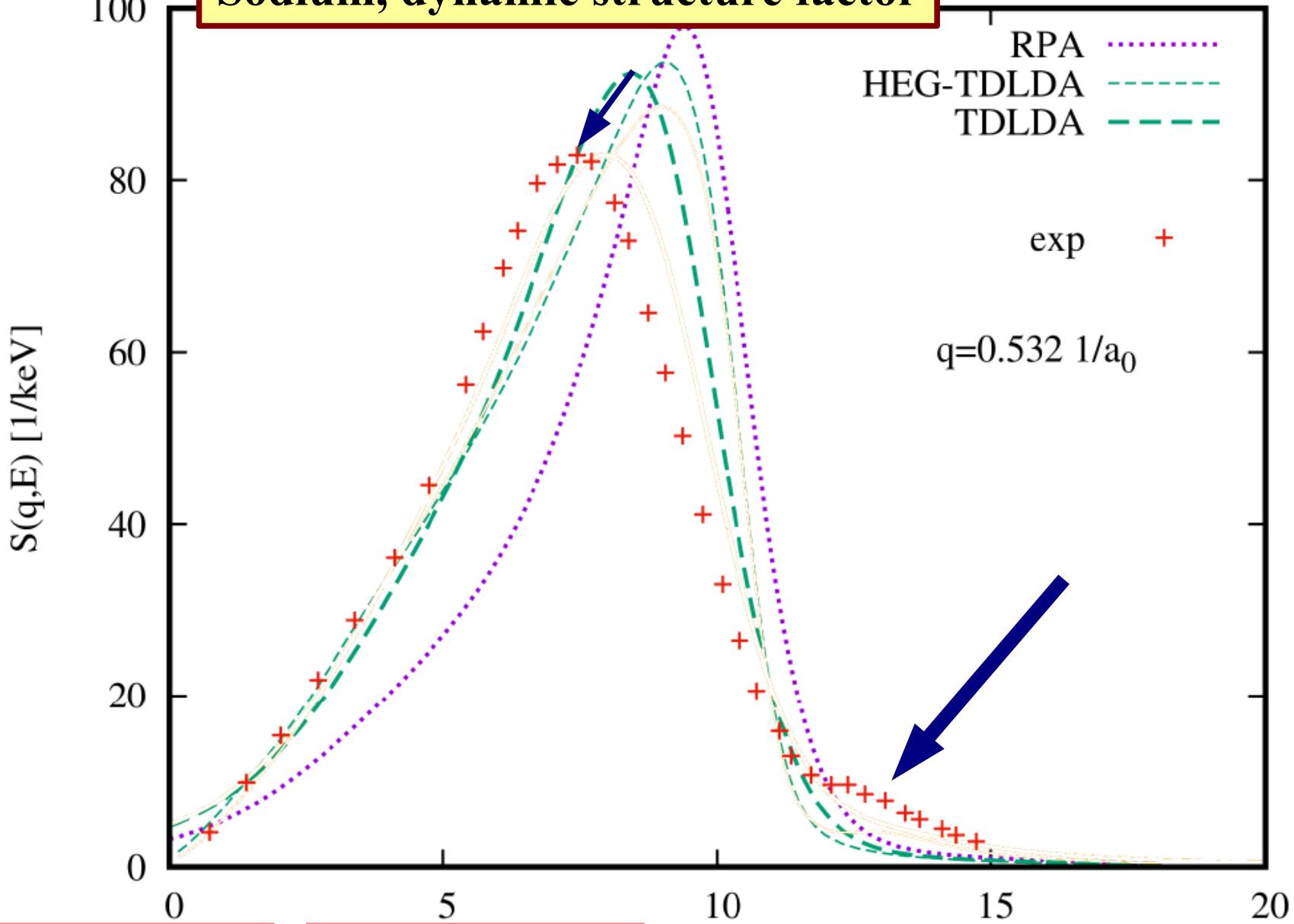
$$S(q,\omega) \sim \text{Im} [\chi(q,\omega)]$$

In TDDFT,

$$\chi(q,\omega) = \chi_{\parallel}(q,\omega) + \chi_{\perp}(q,\omega) \underbrace{\{v(q) + f_{xc}(q,\omega)\}}_{\text{Auxiliary interaction}} \chi(q,\omega)$$

(Matrices in  $G, G'$ )

# Sodium, dynamic structure factor



→ As a model system, we stay with the HEG

$v_{xc}$  in the HEG from QMC (Ceperley and Alder)

But  $f_{xc}$  ?

**Martin Panholzer** following

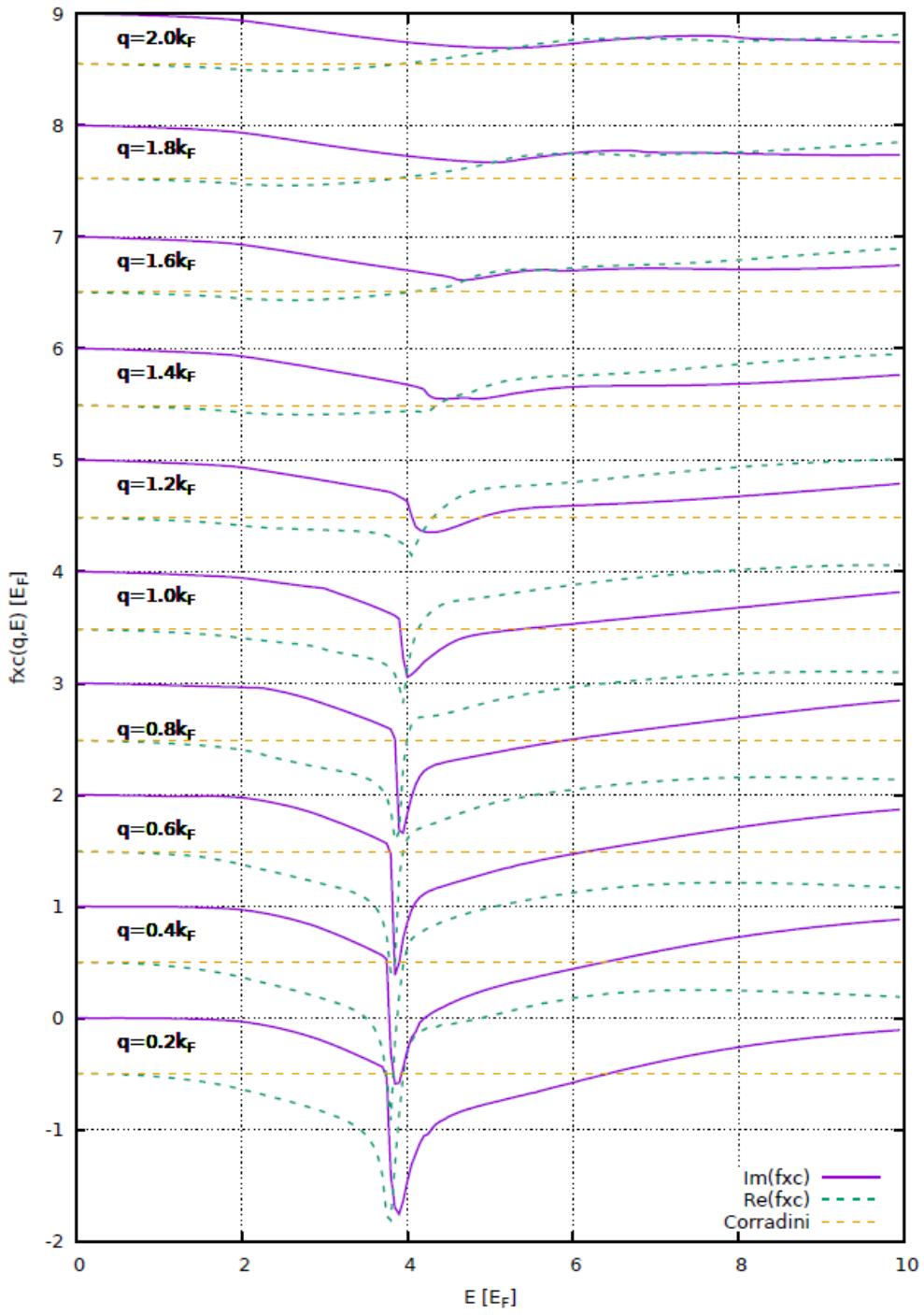
H. M. Boehm, R. Holler, E. Krotscheck, and M. Panholzer,  
Phys. Rev. B 82, 224505 (2010)

→ Calculate  $\chi$  in the HEG:

- action with Jastrow wavefunction
- linear response
- selected number of excitations
- $S(q)$  from QMC

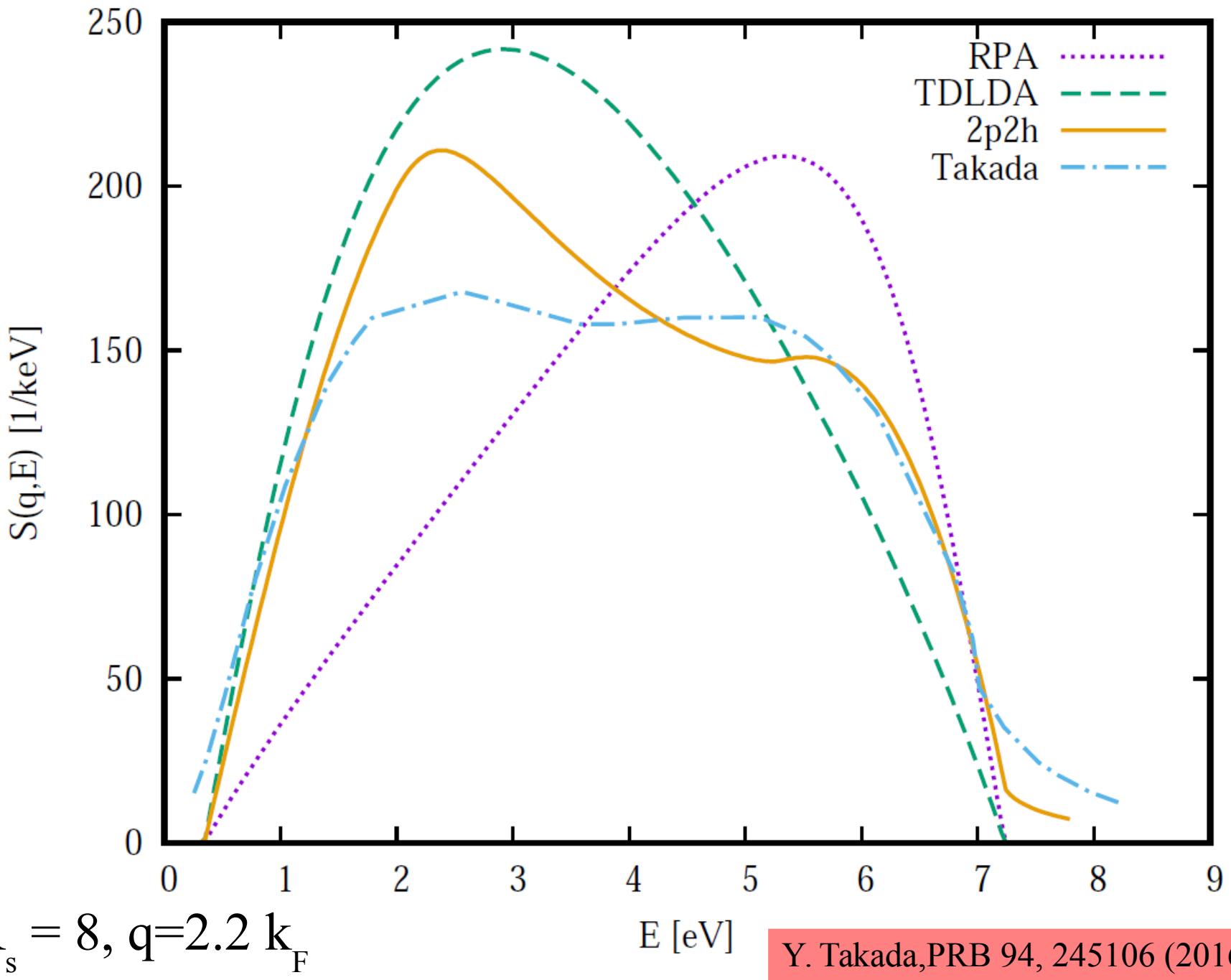
→ Calculate  $f_{xc}$  in the HEG by inverting  $\chi = \chi_0 + \chi_1 [v + f_{xc}] \chi$

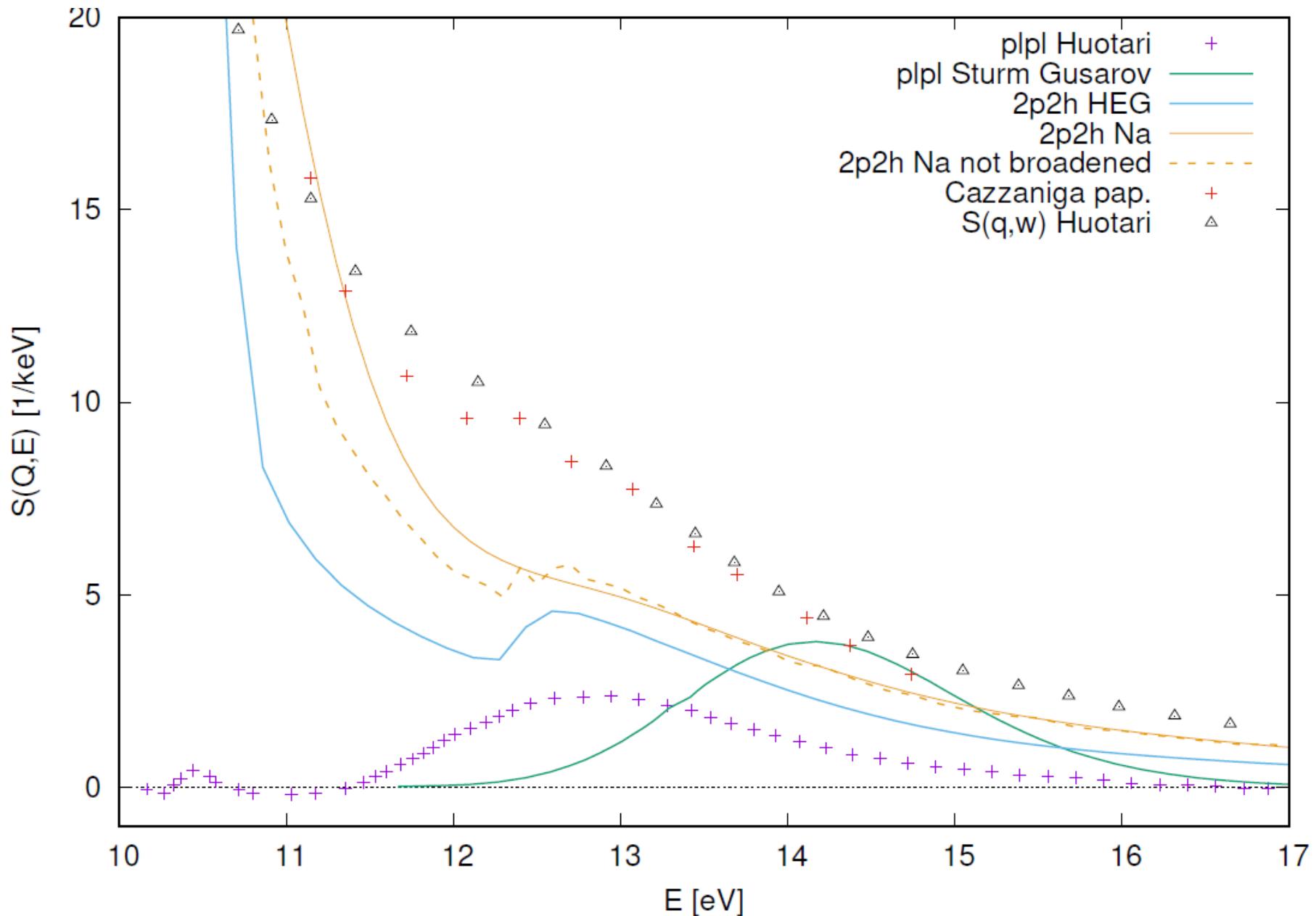
# HEG $f_{xc}$



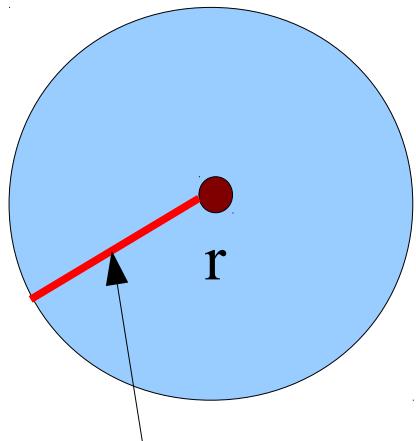
Static: M. Corradini, R. Del Sole,  
G. Onida, and M. Palummo,  
Phys. Rev. B 57, 14569 (1998).

Dynamic: Martin Panholzer et al.





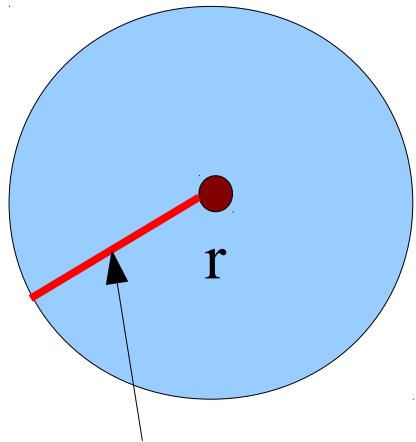
$$f_{xc}(r, r', \omega)$$



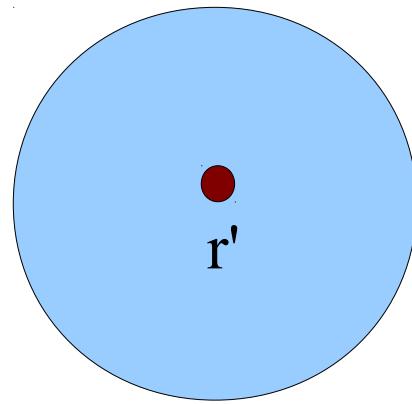
$$1.6 r_s$$

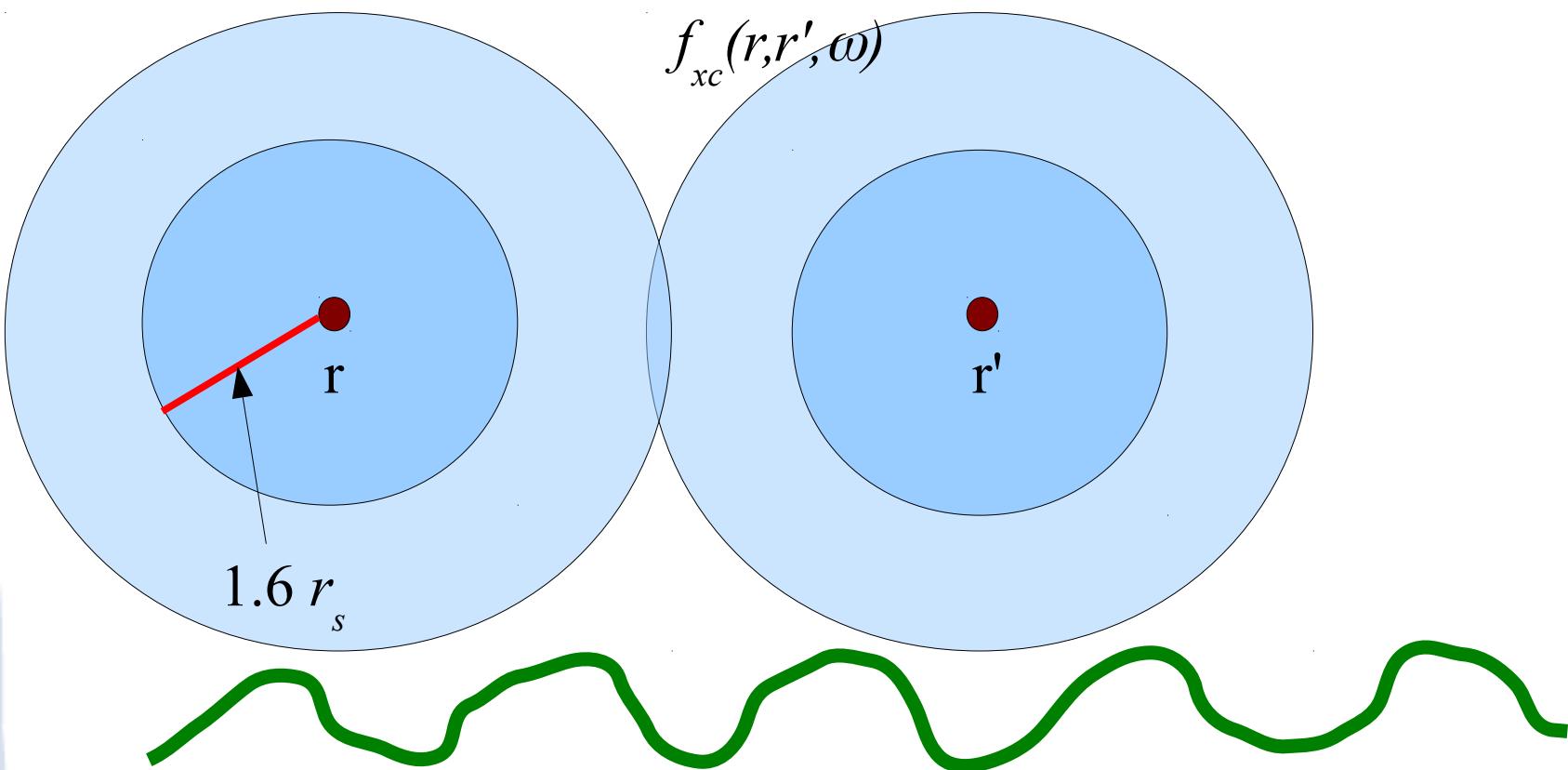
O. Gunnarsson, M. Jonson, and B. Lundqvist,  
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$$f_{xc}(r, r', \omega)$$



$$1.6 r_s$$



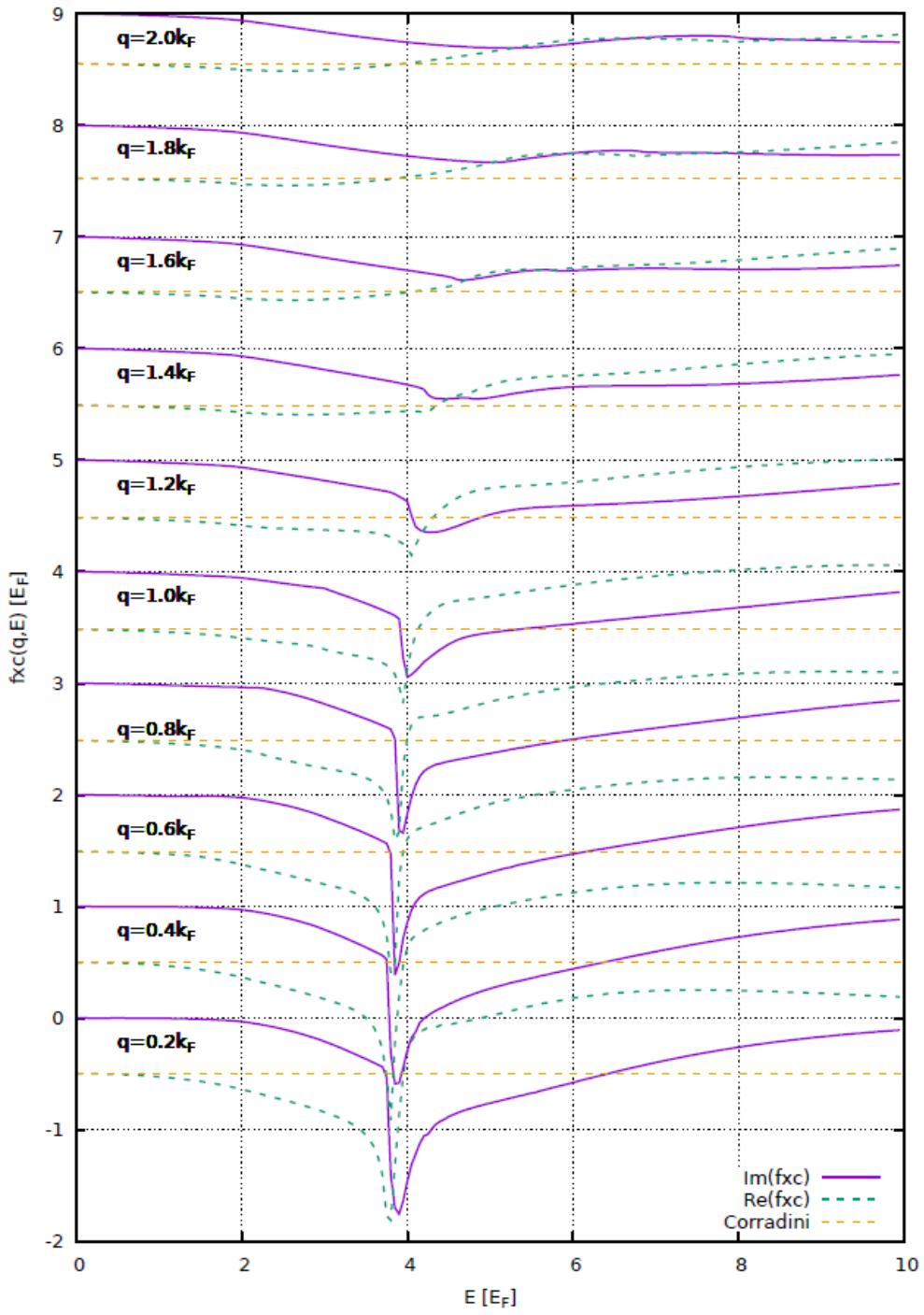


Interatomic distances:     $\text{Na} = 1.75 r_s$      $\text{Si} = 2.2 r_s$

→ Mean Density Approximation

See also V. U. Nazarov, G. Vignale, and Y.-C. Chang,  
Phys. Rev. Lett. 102, 113001 (2009).

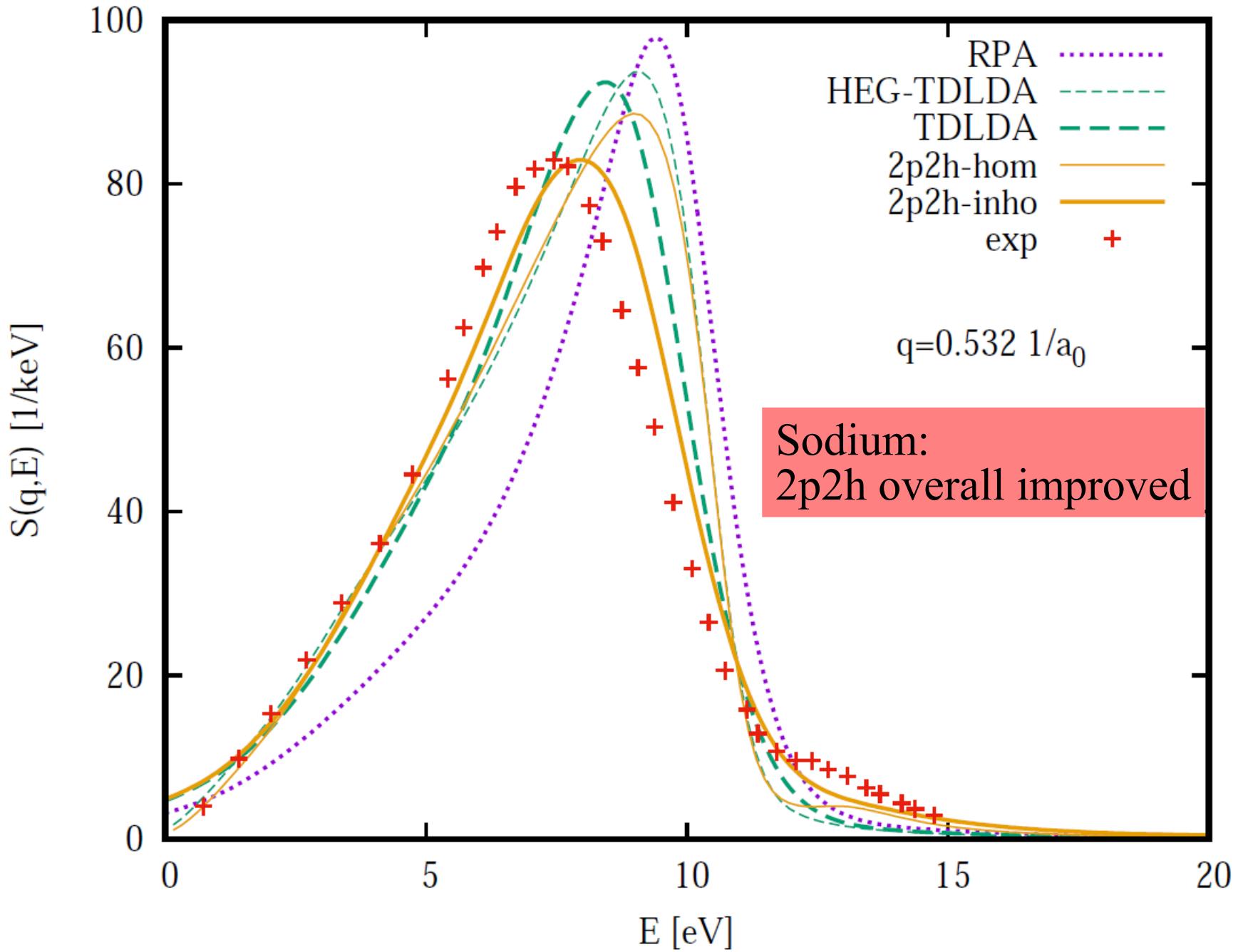
# HEG $f_{xc}$

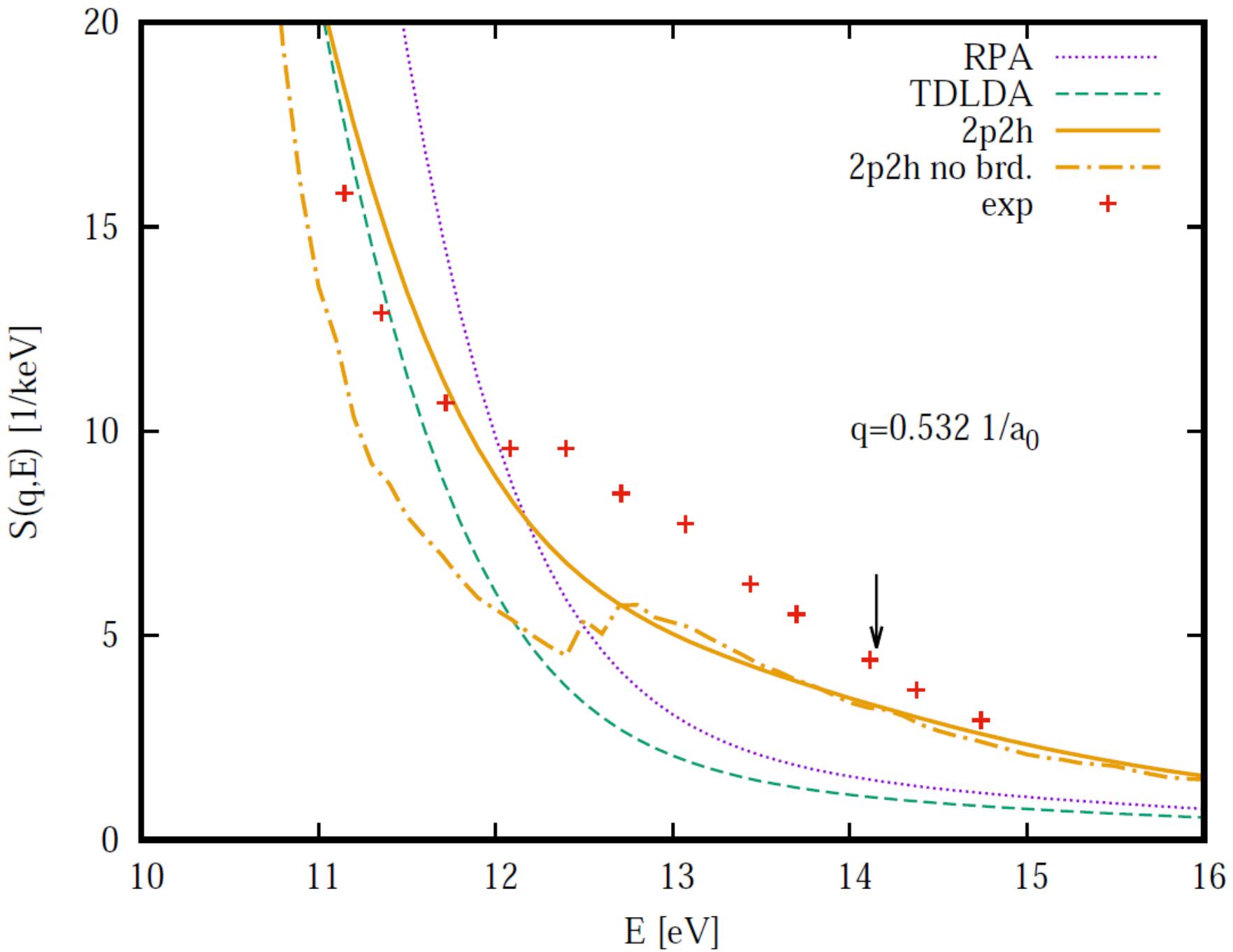


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Phys. Rev. B 57, 14569 (1998).

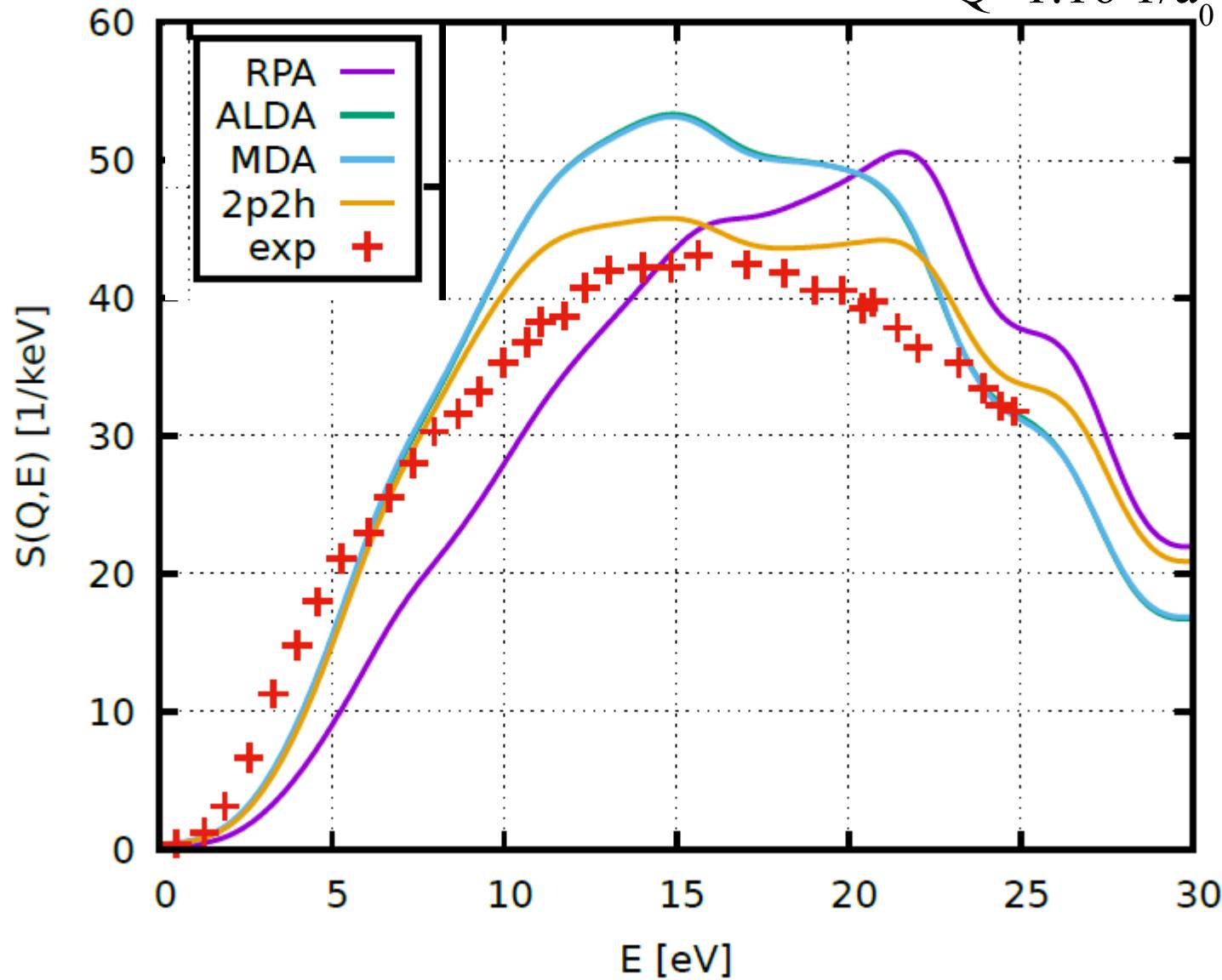
Dynamic: Martin Panholzer et al.

Connector for  $f_{xc}(r,t;r',t')$ :  
“mean density approximation”

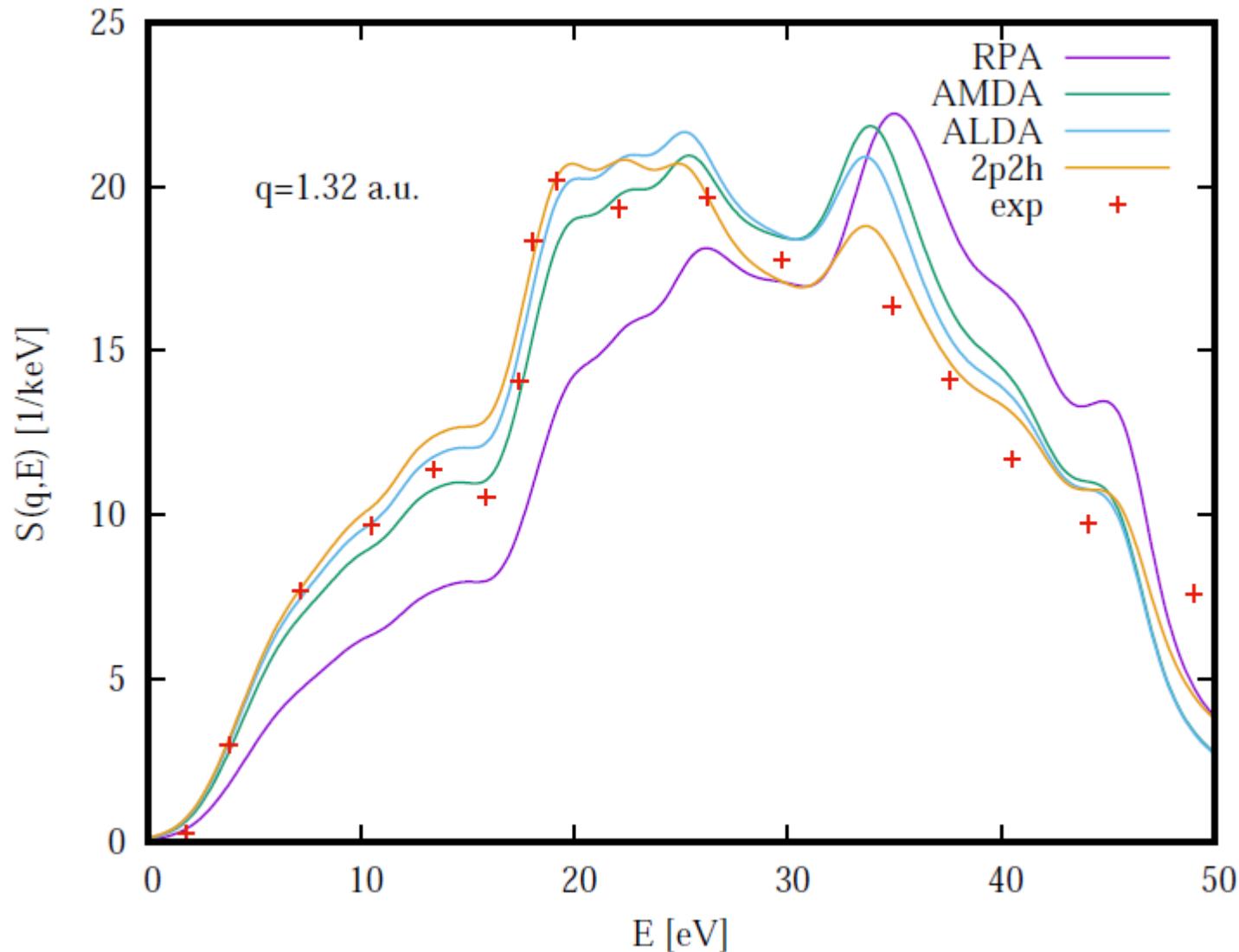




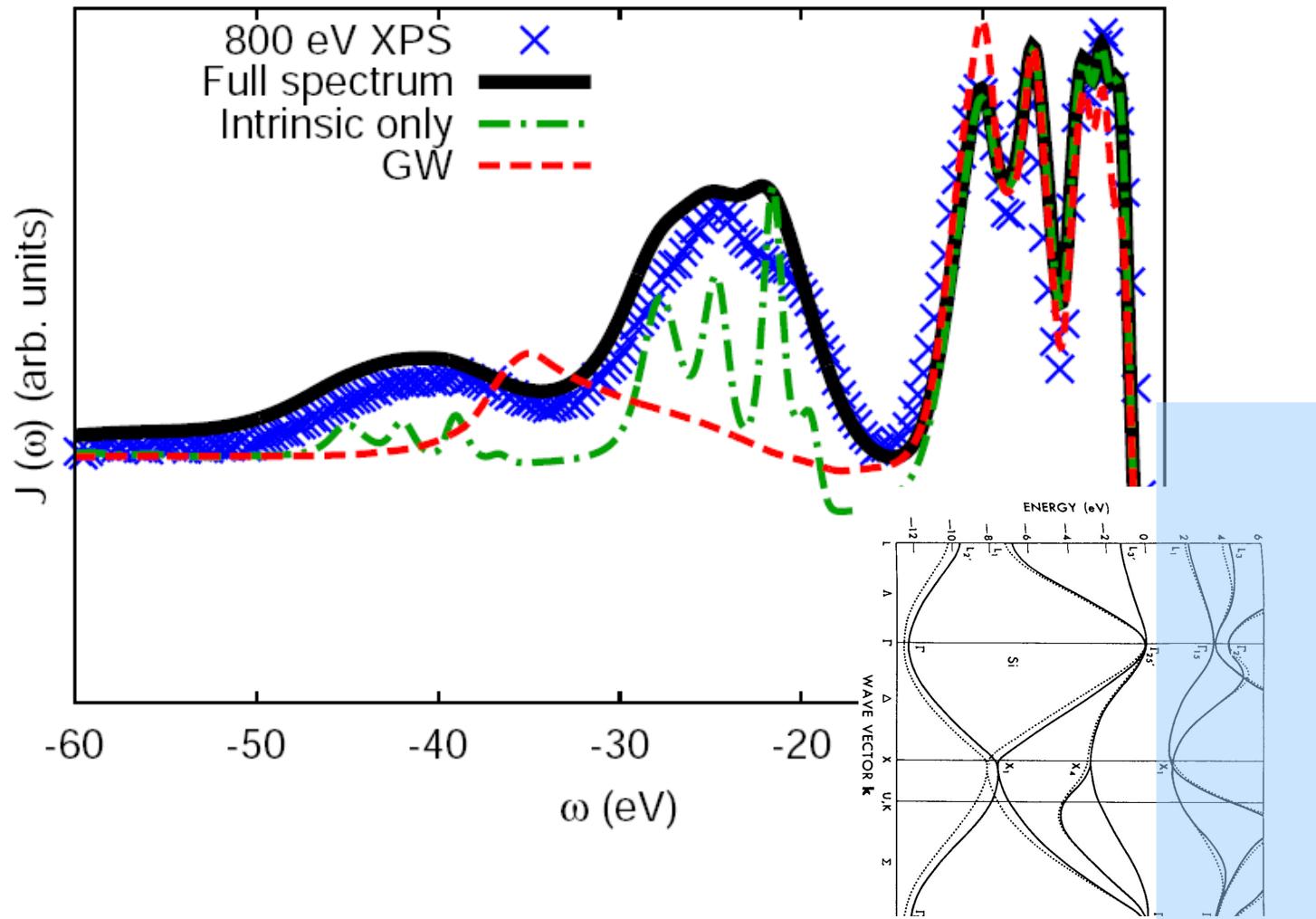
$Q=1.16 \frac{1}{a_0}$



# Silicon



# → Connector Theory for one-body spectral functions



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

M. Guzzo et al., PRL 107, 166401 (2011)

Usually from GW, or similar

$$G(\mathbf{r}, \mathbf{r}', \omega) = G_0(\mathbf{r}, \mathbf{r}', \omega) + G_0(\mathbf{r}, \mathbf{r}_1, \omega) \underbrace{\Sigma(\mathbf{r}_1, \mathbf{r}_2, \omega)}_{\text{Non-local, complex self-energy}} G(\mathbf{r}_2, \mathbf{r}', \omega)$$

Non-local, complex self-energy

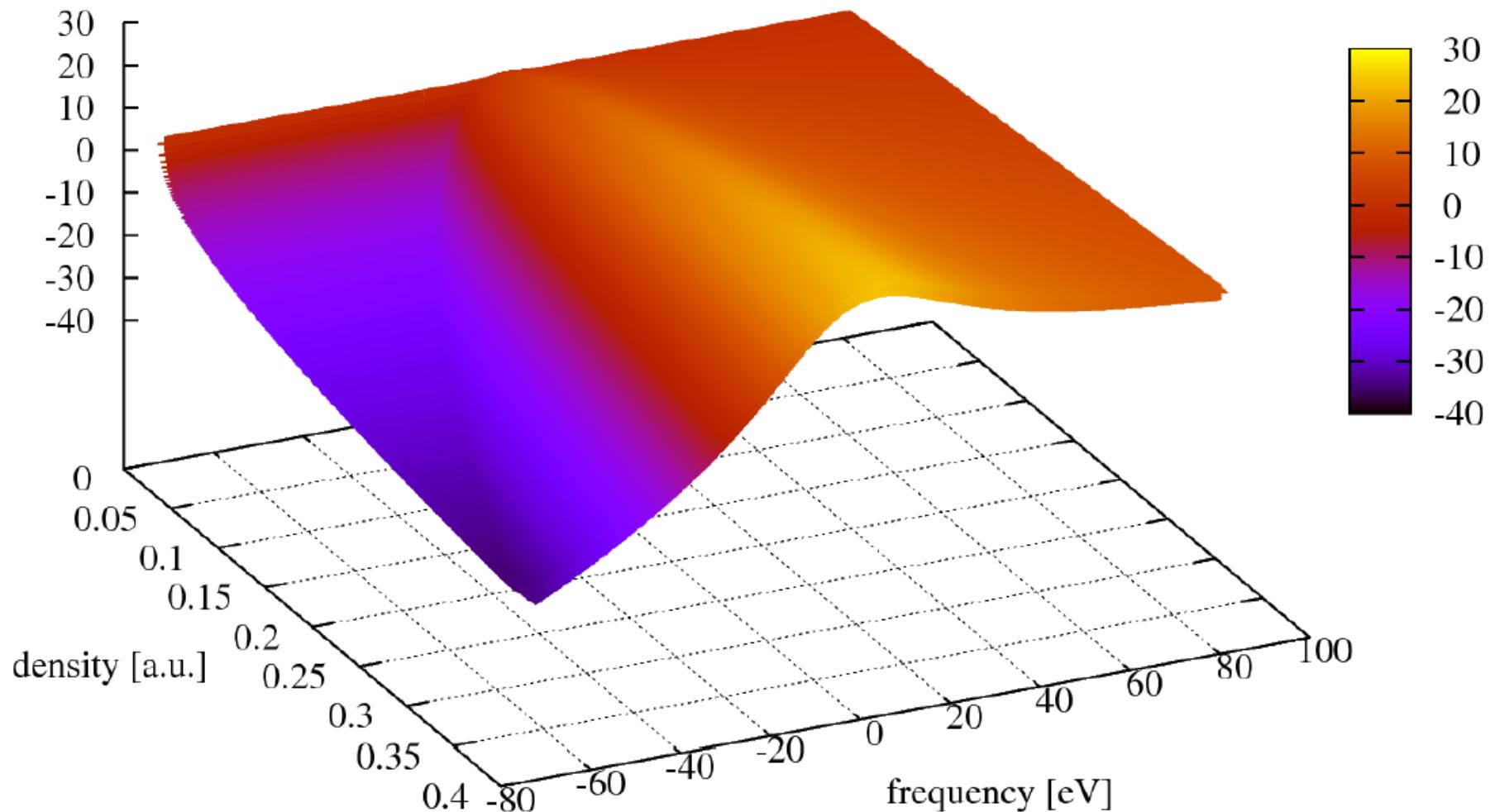
$$A_{\ell\ell}(\omega) = \frac{1}{\pi} |\text{Im } G_{\ell\ell}(\omega)| \quad \text{ARPES: } \ell = \mathbf{k}$$

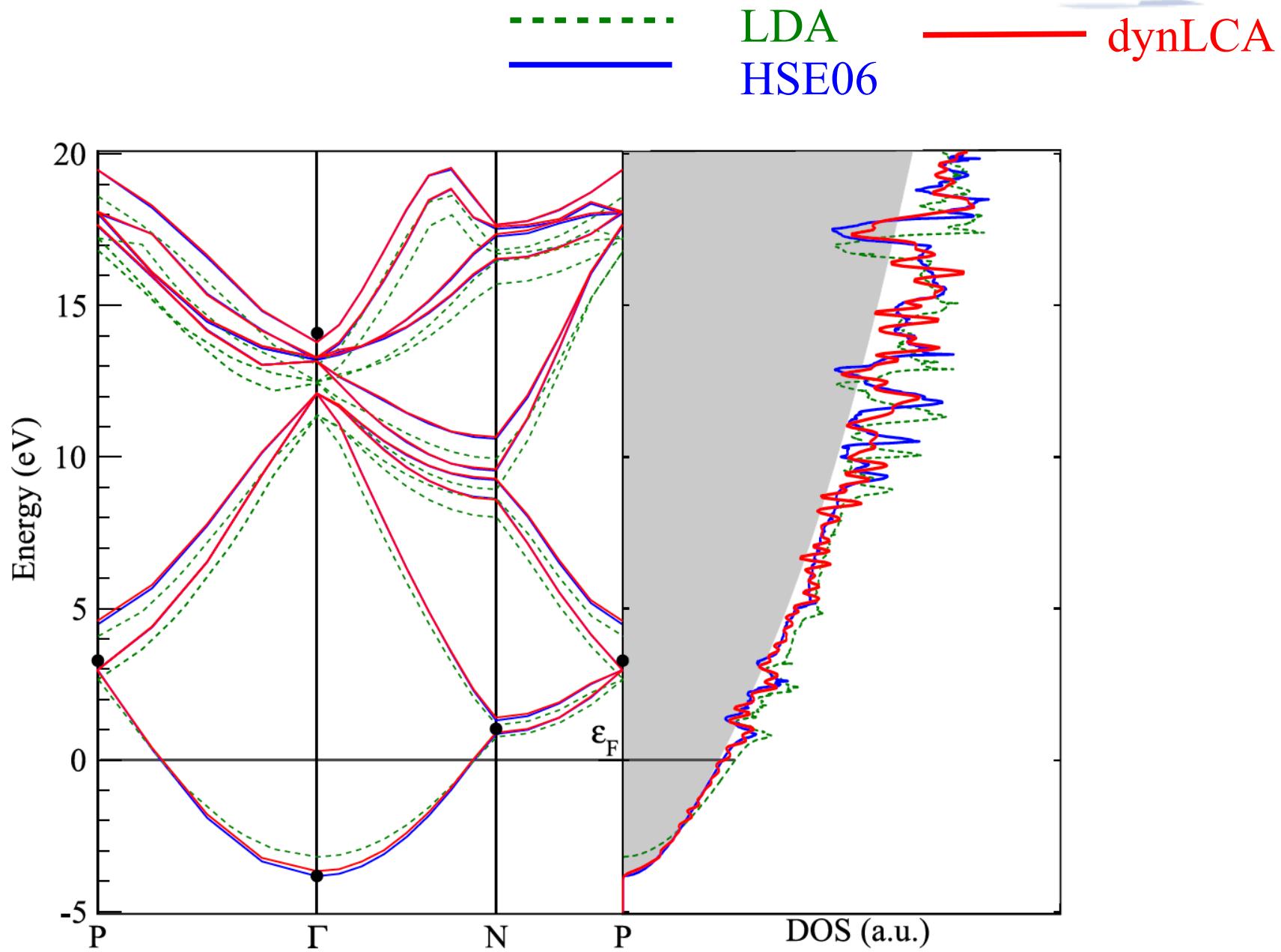
$$\text{PES: } A(\omega) = \sum_{\ell} A_{\ell\ell}(\omega) = \frac{1}{\pi} \int d\mathbf{r} |\text{Im } G(\mathbf{r}, \mathbf{r}, \omega)|$$

$$n(\mathbf{r}) = \int_{-\infty}^{\mu} d\omega A(\mathbf{r}, \mathbf{r}, \omega)$$

Only a part of  $G$  needed → can we make a simpler auxiliary system?  
YES:  $v_{SF}(\mathbf{r}, \omega)$  (see M. Gatti et al., PRL 99 057401 (2007))

$v_{SF}(\mathbf{r}, \omega)$  from  $\Sigma(\mathbf{r}, \mathbf{r}')$  HSE06       $\rightarrow$  in HEG:  $v_{SF}(\omega)$  from  $\Sigma(\mathbf{r}-\mathbf{r}')$   
(perturbative)

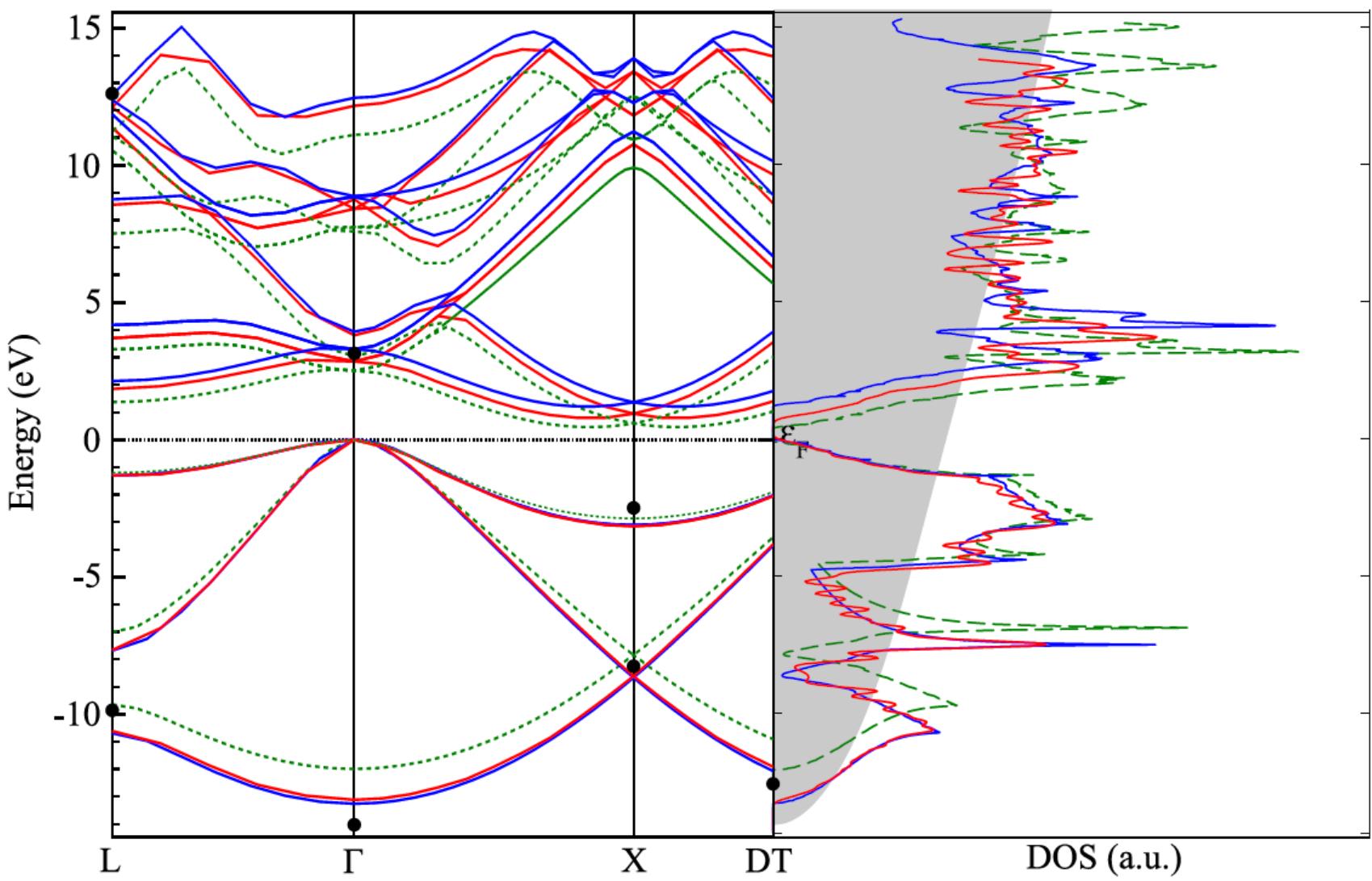




Silicon

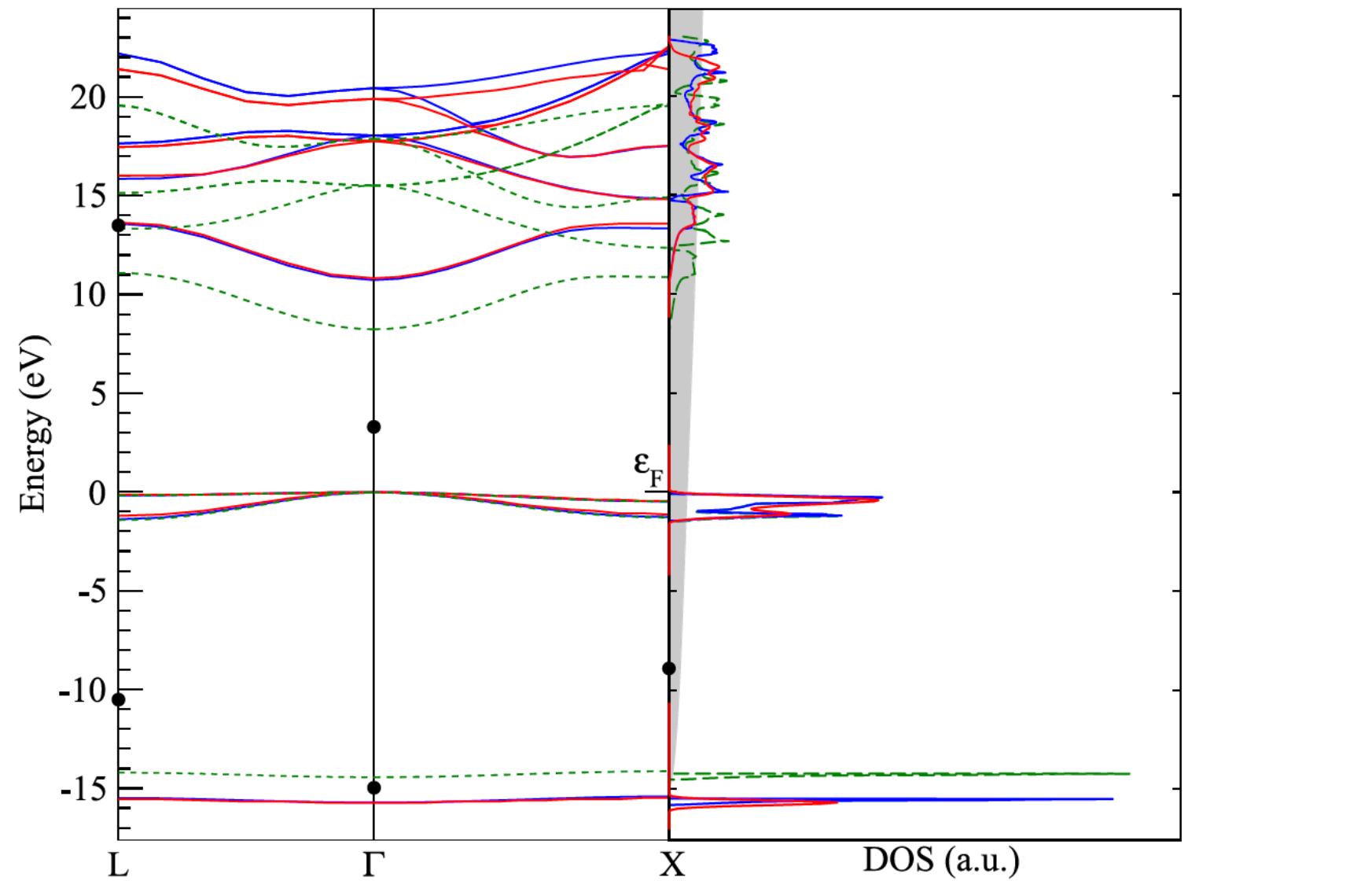
— LDA  
— HSE06

— dynLCA



# Solid Argon

— LDA  
— HSE06



→ Goal and problem

→ Recycling I: → Cumulants

- \* *satellites in the one-body spectral function*
- \* *satellites in the two-body spectral function*

→ Recycling II: → Connector Theory

- \* *the dynamic structure factor*
- \* *the one-body spectral function*

→ Conclusions and outlook

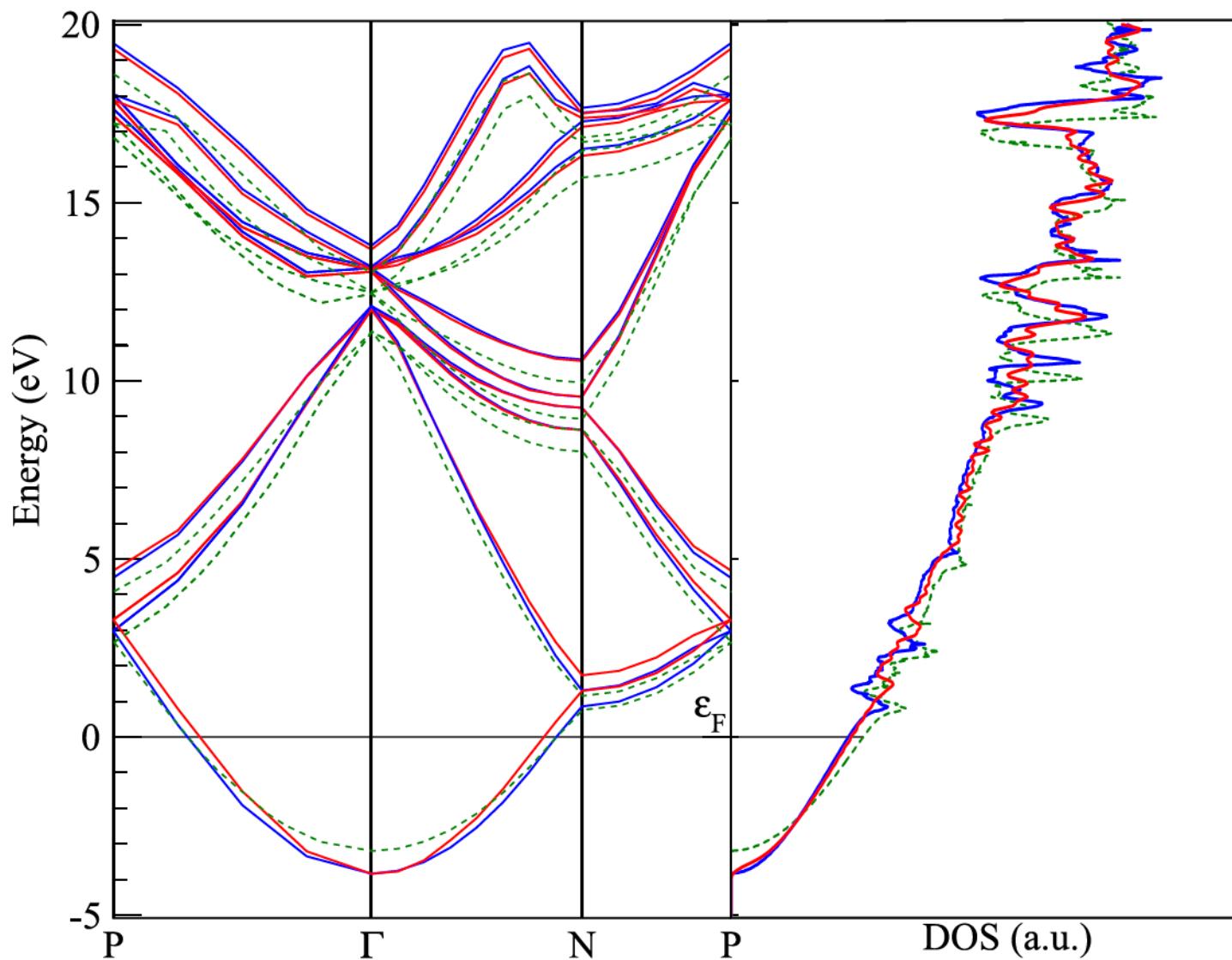
G. Lani, P. Romaniello, and L. Reining, New J. Phys. 14, 013056 (2012); J.A. Berger et al., New J. Phys. 16, 113025 (2014); A. Stan, et al., New J. Phys. 17, 093045 (2015);

JS Zhou, et al., J. Chem. Phys. 143, 184109; JS Zhou, M Gatti, JJ Kas, JJ Rehr, L Reining, Phys. Rev. B 97, 035137 (2018);

M Vanzini, L Reining, M Gatti, arXiv:1708.02450; M Panholzer, M Gatti, L Reining; arXiv:1708.02992.

# Sodium as a test case

— LDA  
— HSE06



Connector:

$$v_{SF}(\mathbf{r}, \omega) =$$

$$v_{n^h=n(\mathbf{r})}^h \left[ \frac{\omega_P(n(\mathbf{r}))}{\omega_P(\bar{n})} \left( \omega - v_{KS}(\mathbf{r}) + v_{KS}^h[\bar{n}] \right) + v_{xc}(\mathbf{r}) - v_{xc}^h[\bar{n}] \right]$$

LDA

Energy scale

dynLDA

Alignment of energies

In the HEG,  $k \longleftrightarrow \omega$

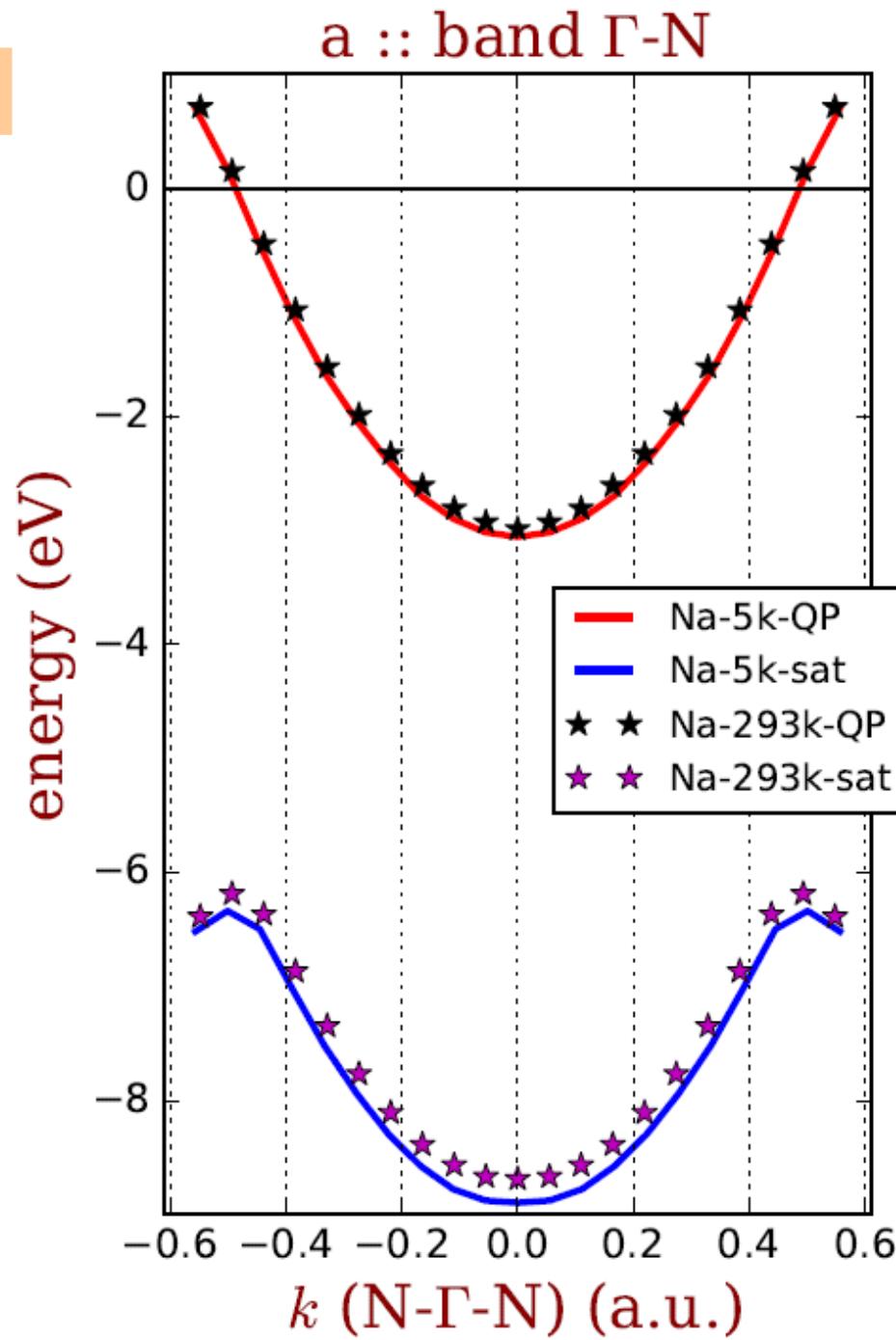
→ we can correct the b.s. by  $\Delta(\omega)$  while keeping  $A(\omega)$  the same  
(but change way to calculate it)

Then use  $v_{SF}^h(\omega) \rightarrow v_{SF}^h(\omega) - \Delta^h(\omega)$

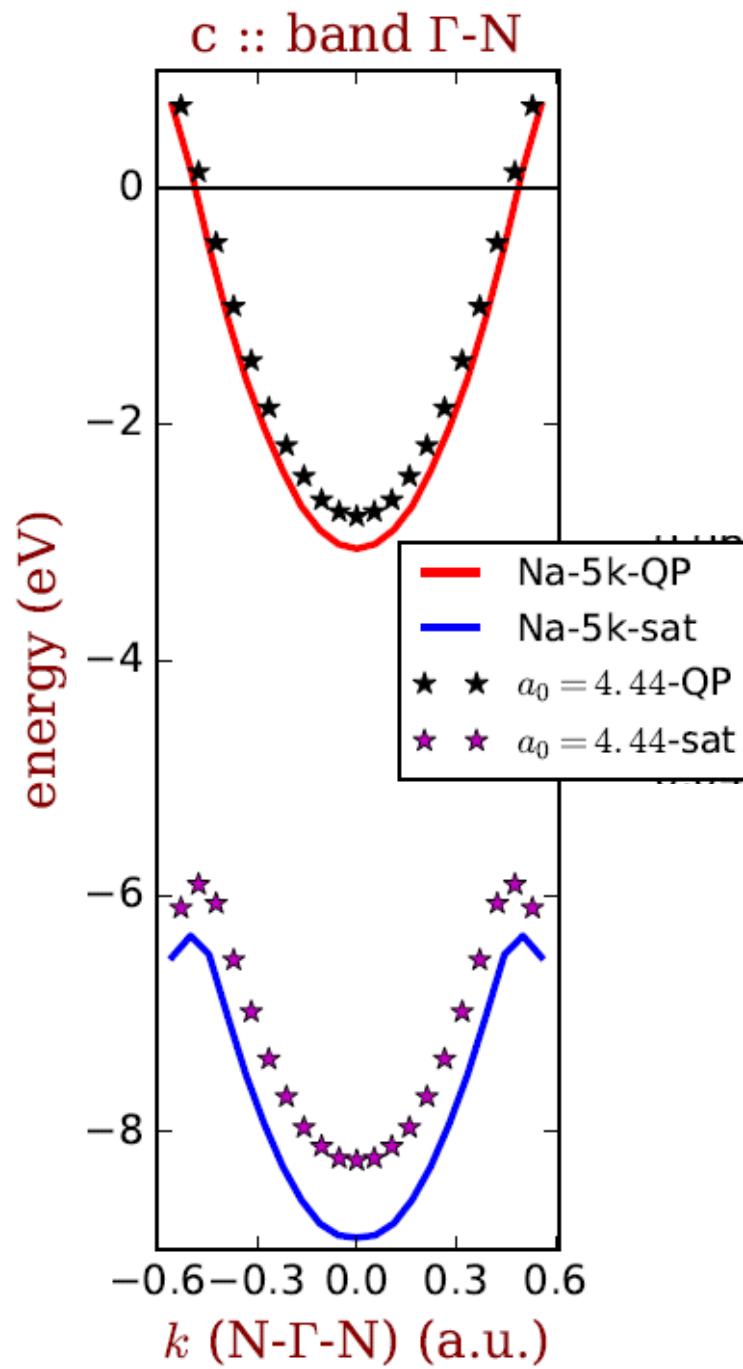
in

$$v_{SF}(\mathbf{r}, \omega) = \\ v_{n^h=n(\mathbf{r})}^h \left[ \frac{\omega_P(n(\mathbf{r}))}{\omega_P(\bar{n})} \left( \omega - v_{KS}(\mathbf{r}) + v_{KS}^h[\bar{n}] \right) \right] \\ + v_{xc}(\mathbf{r}) - v_{xc}^h[\bar{n}]$$

## Lattice Constant



# Lattice Constant



# Quasi-particles and satellites from a direct approach to the calculation of many-body Green's functions

- “Dynamical” correlation effects from Green's functions
- Details of screening needed!
- Screening beyond RPA: don't work too much!
  - Connector Theory
- Connector Theory for spectral functions
- Conclusions and outlook

# The great idea: local density approximation

1. Near-sightedness principle:

$$v_{xc}[n](r) \rightarrow v_{xc}(n(r), r)$$

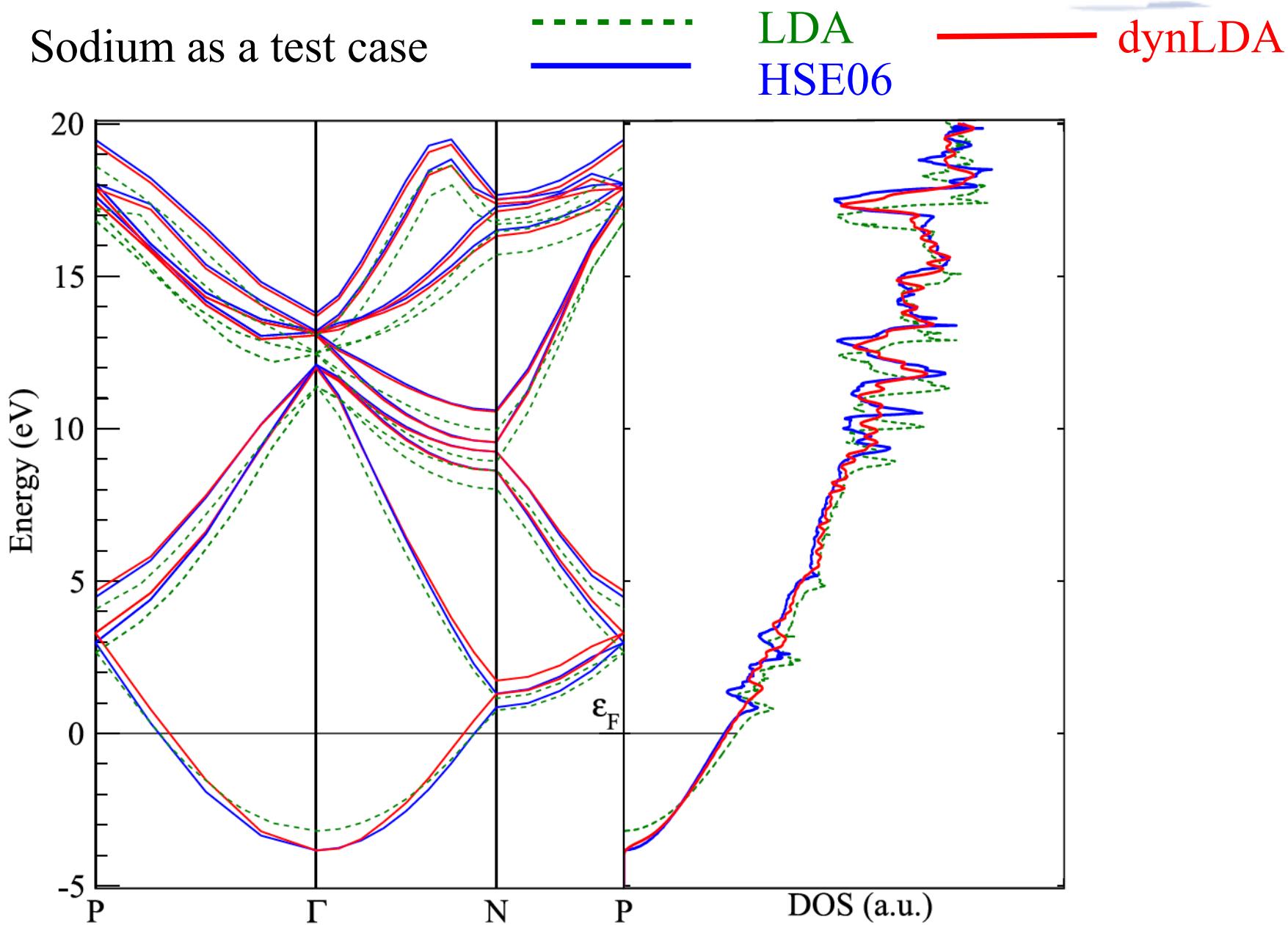
2. Near-sightedness principle:

Locally as in the HEG,

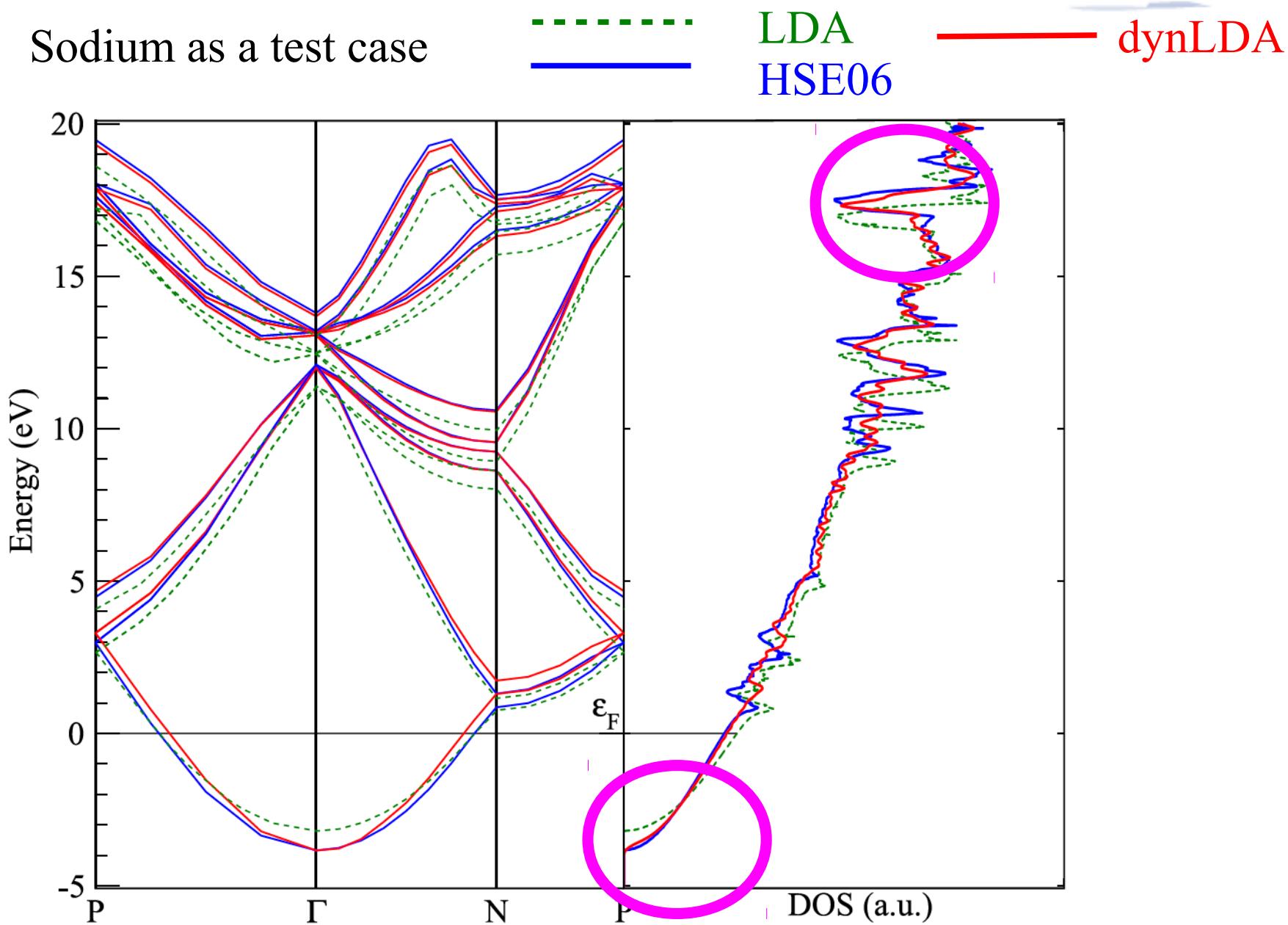
$$v_{xc}(n(r), r) \rightarrow v_{xc}^{\text{HEG}} \quad \text{with } n=n(r)$$

**Calculated super well and once forever!!!**

# Sodium as a test case

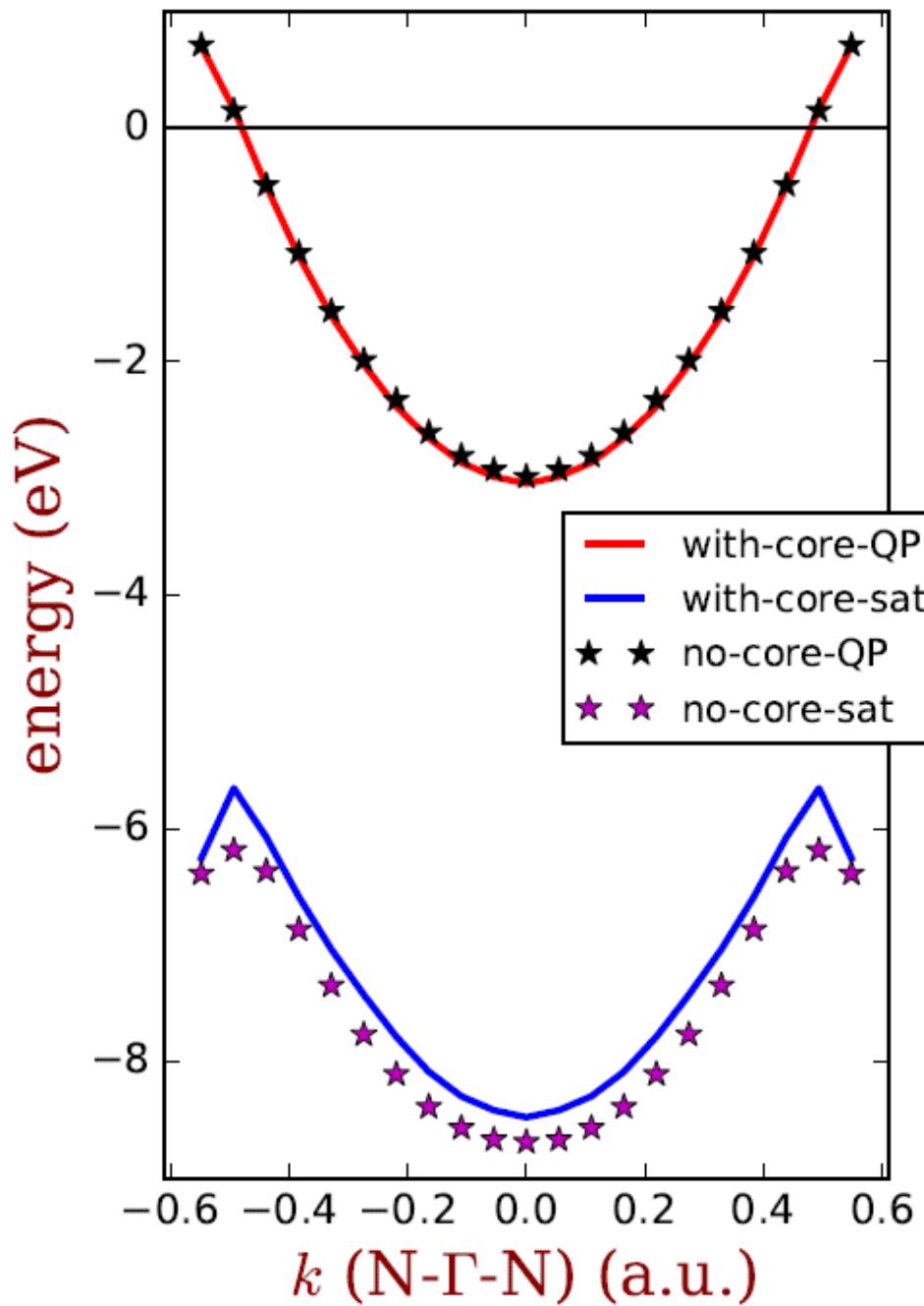


# Sodium as a test case

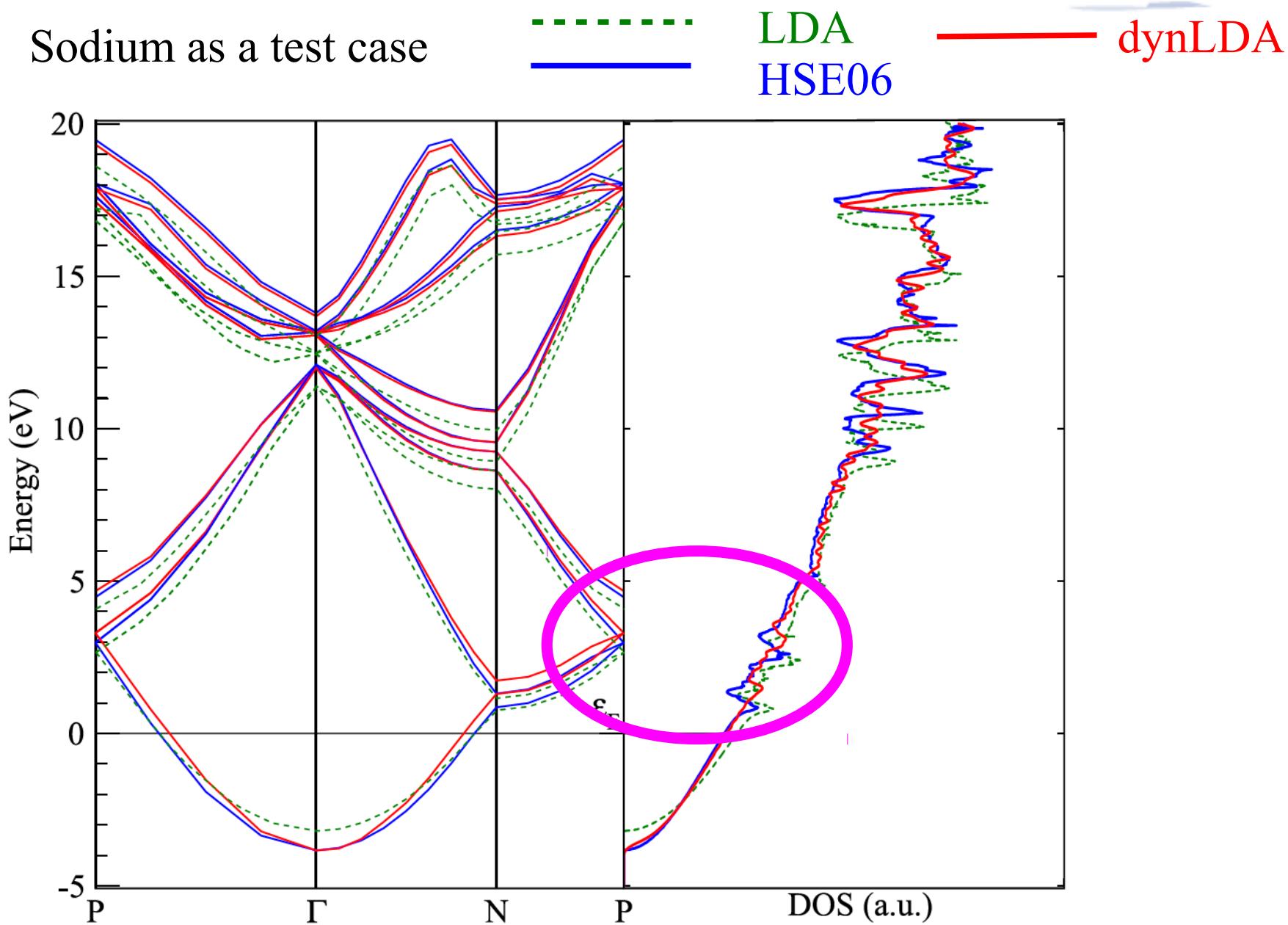


## Core polarization

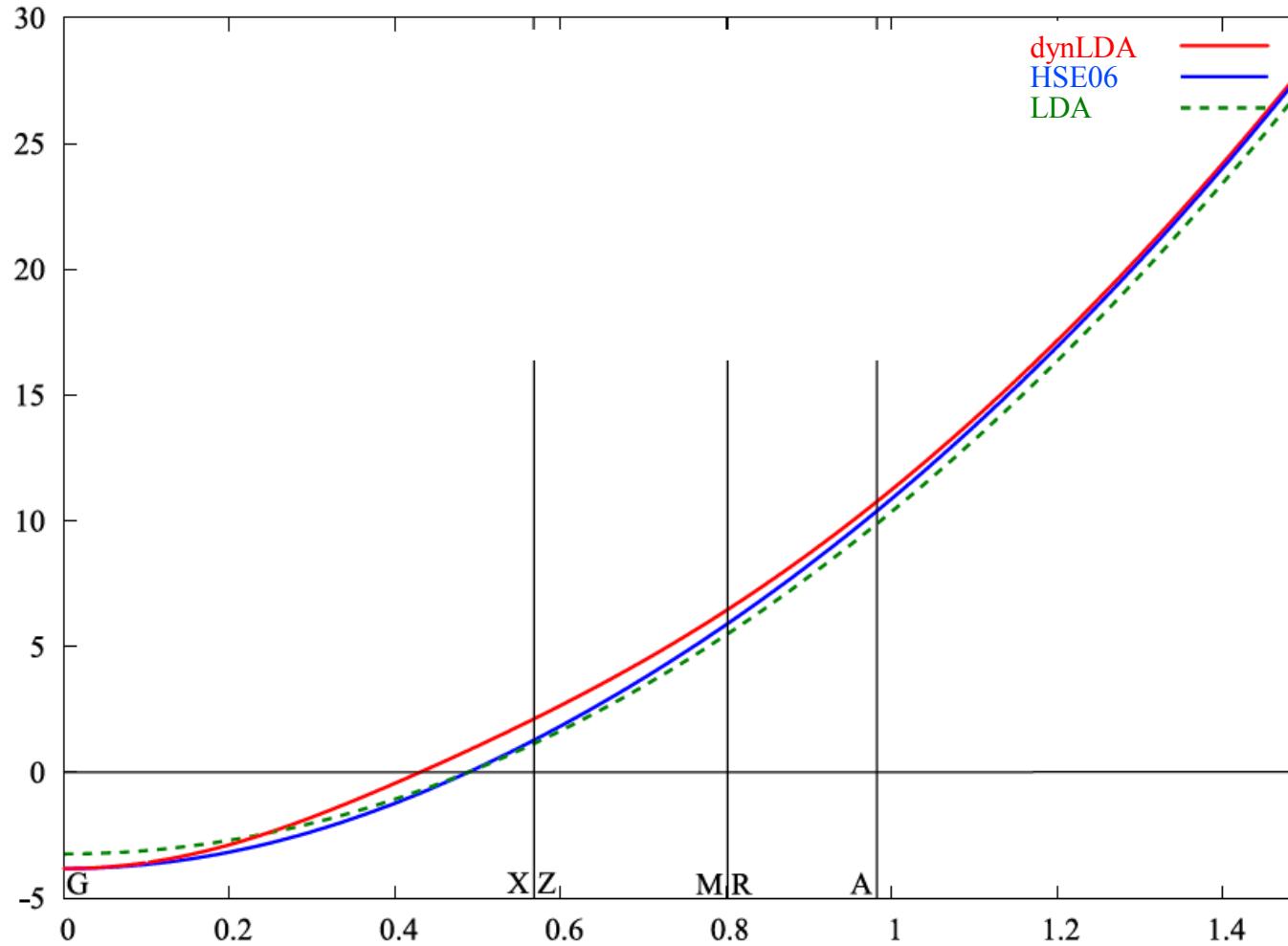
c :: band  $\Gamma$ -N



# Sodium as a test case



$$A(\omega) = \sum_{n\mathbf{k}} \delta(\omega - \varepsilon_{n\mathbf{k}}^{SF}(\omega)) = \sum_{n\mathbf{k}} \delta(\omega - \varepsilon_{n\mathbf{k}}^{HSE06})$$



In HEG by definition: same DOS, although b.s. different!!!

## → The one-body Spectral function

- Real, local and frequency dependent “HSE06-potential” tabulated in HEG
- Can be used with simple connector; CPU gain >> factor 10

*For quite homogeneous and for quite local systems:*

- Reproduce integrated spectral function very well
- Reproduce also the band structure very well

*For covalent semiconductor:*

- Reproduce band width in integrated spectral function very well
- Correct about 30% of KS-LDA gap error
- Corresponding quality of the band structure

→ Why are we here?

Calculate few systems well

**Connector**

→ Connector theory for observables

Use to study many

→ The dynamic structure factor

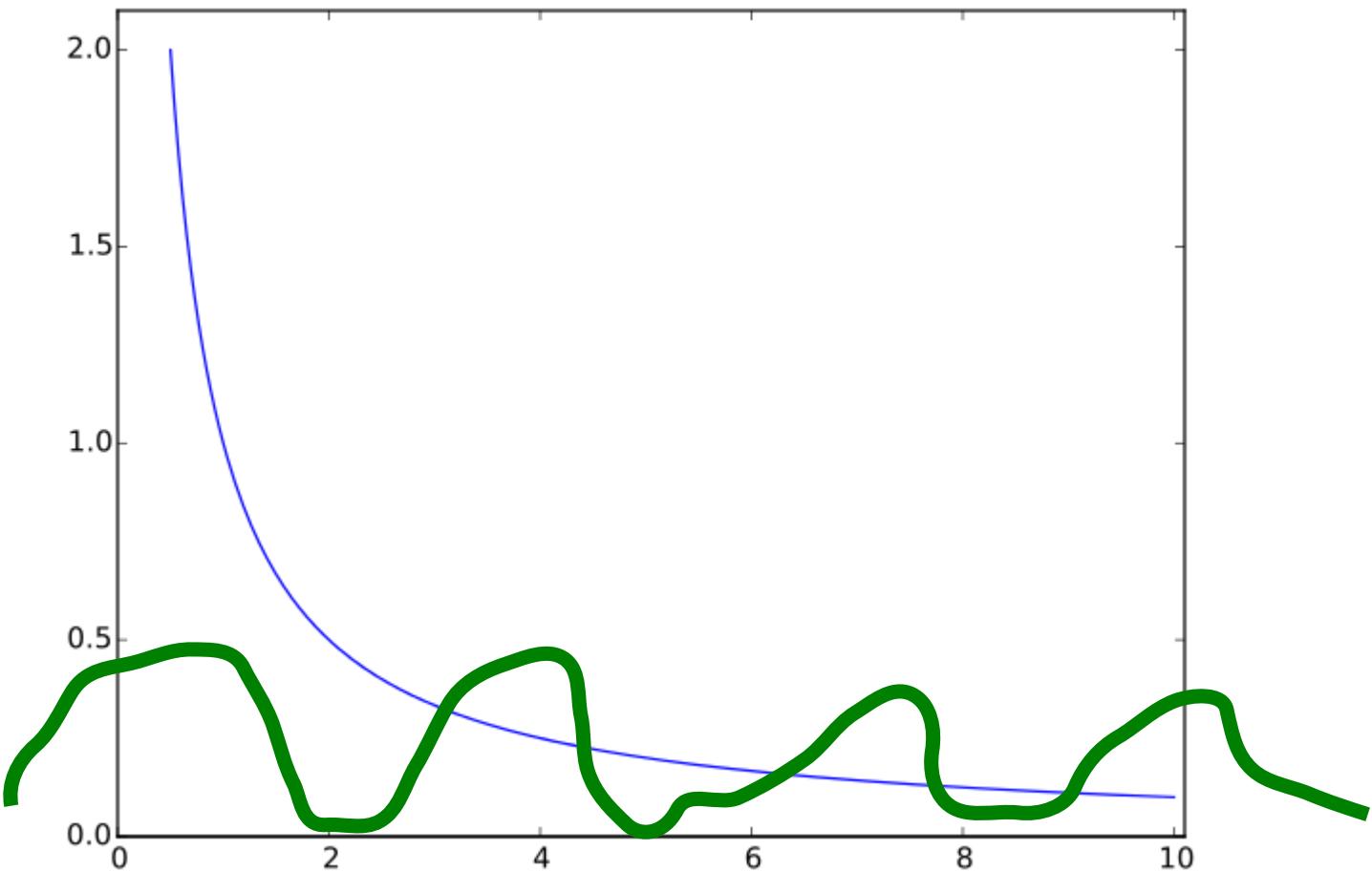
Non-local, non-adiabatic  $f_{xc}$

→ The one-body spectral function

Local, real,  $\omega$ -dep. Potential  
Advanced connector

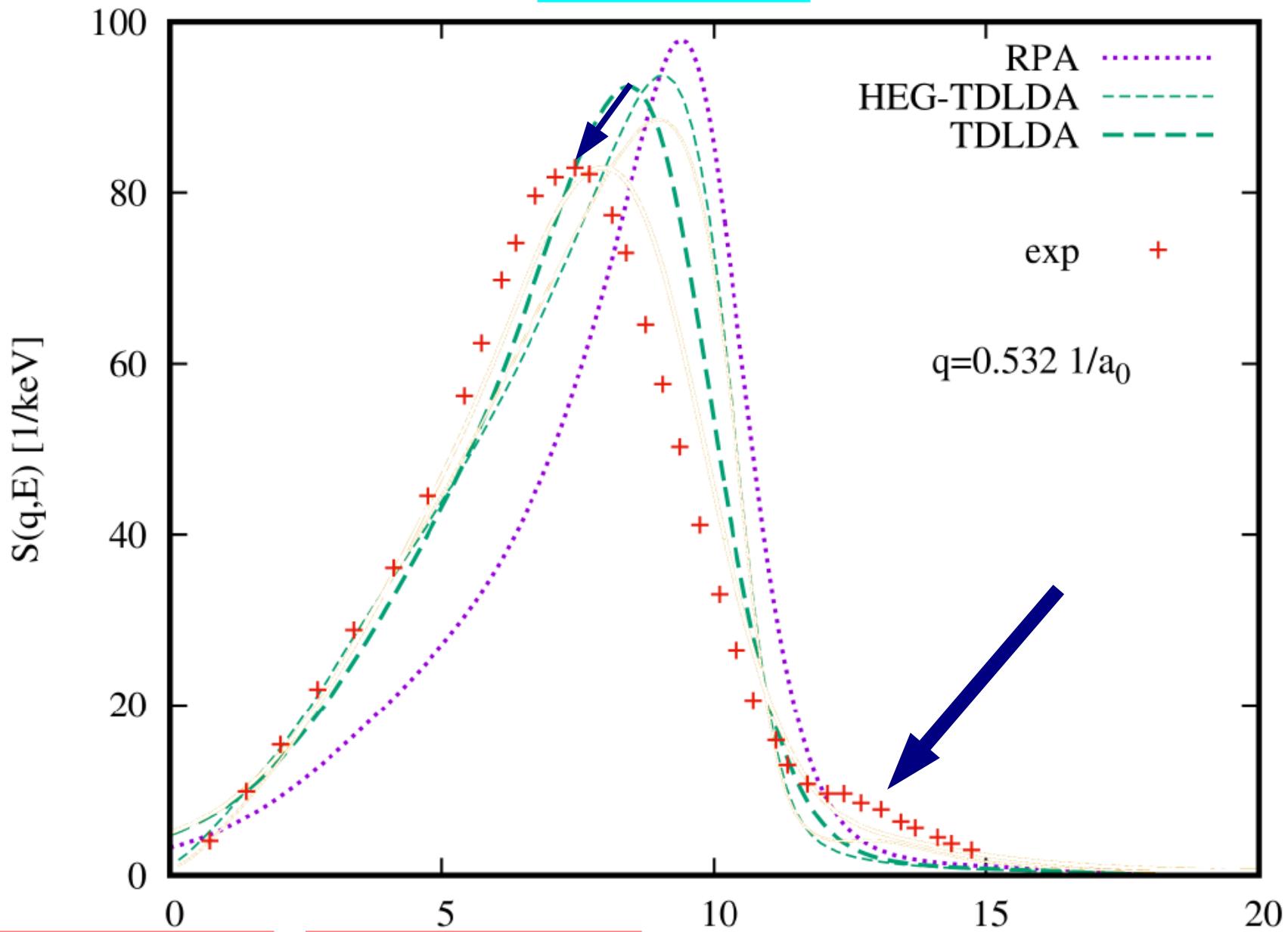
→ New auxiliary systems

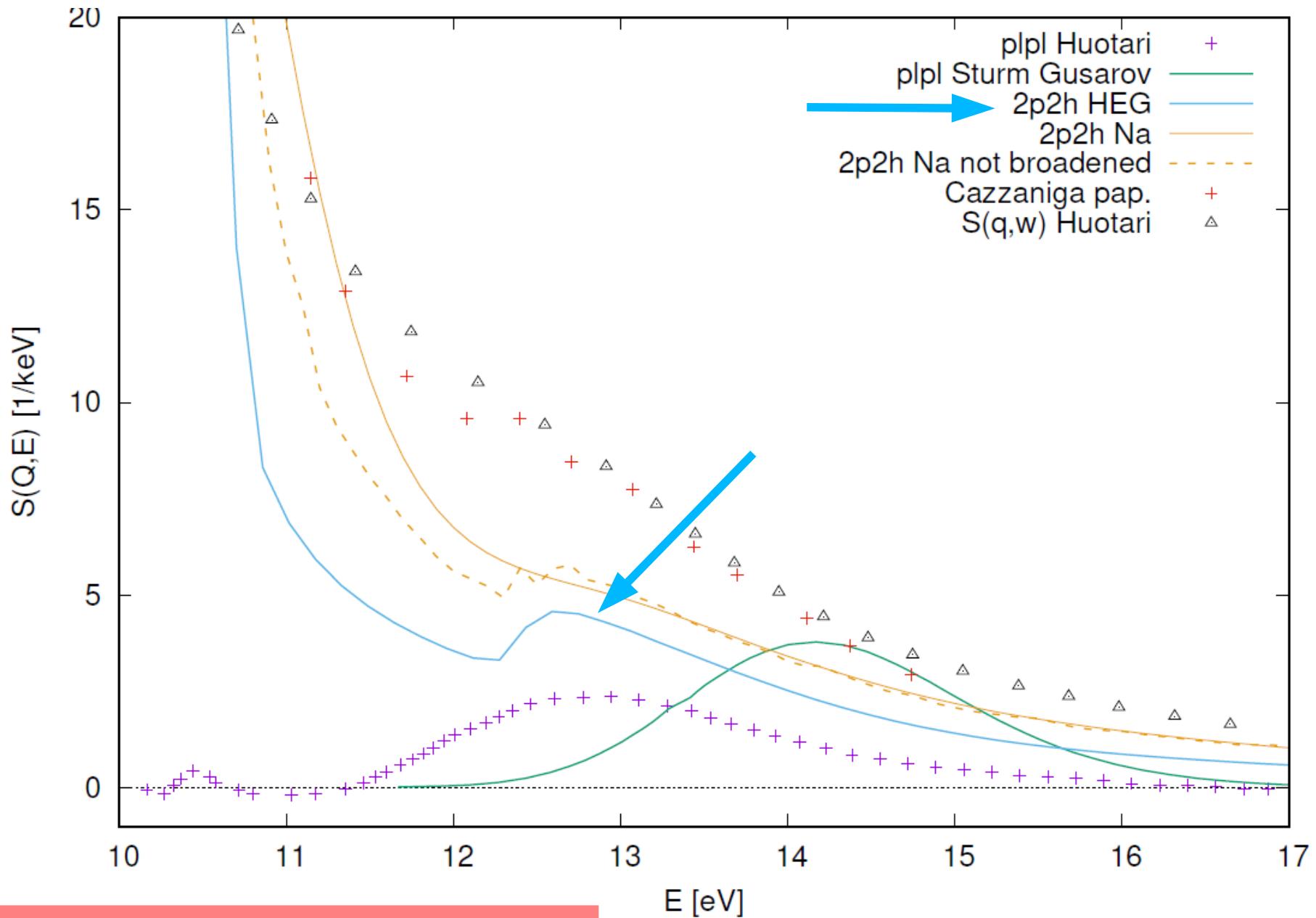
plus new connectors: a very promising way to go!

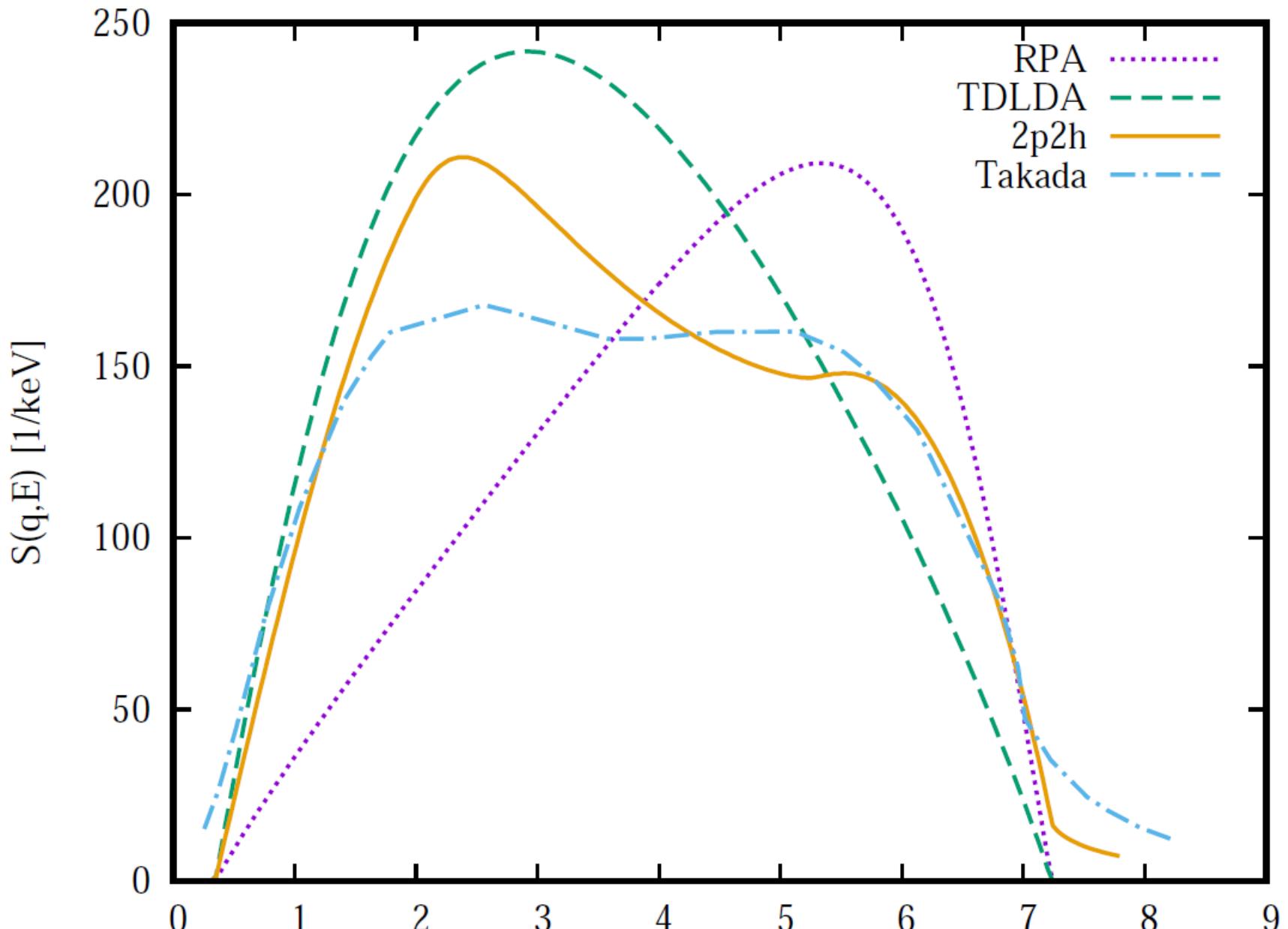


We know that  $f_{xc}$  can often be taken to be quite smooth (head only) →  
Must average around  $r, r'$ .  
If the density variation is fast on the scale of  $r - r'$  → **MDA**

# IXS-Sodium







$r_s = 8, q=2.2 k_F$

$E$  [eV]

See Y. Takada, PRB 94, 245106 (2016)

## → Connector Theory

$$V^{\text{real}}(x, P) = V^{\text{model}}(y, P_c(y, x, P)) \rightarrow \text{Model must span real range}$$

$$P_c(x, y, P) = (V^{\text{model}})^{-1}(y, V^{\text{real}}(x, P)) \rightarrow P_c \text{ must be allowed value}$$

For example, real and positive if  $P_c = n$

## → Connector Theory: Example

*Target:* Hartree potential of finite system. *Model:* jellium sphere.

$$v_H(\mathbf{r}, [n]) = \int d\mathbf{r}' \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \stackrel{!}{=} n^{hom} \int_R d\mathbf{r}' \frac{1}{|\mathbf{r} - \mathbf{r}'|}$$

$$n^{hom}(\mathbf{r}, [n]) = \int d\mathbf{r}' \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \left/ \int_R d\mathbf{r}' \frac{1}{|\mathbf{r} - \mathbf{r}'|} \right.$$

$$v_H(\mathbf{r}, [n]) = v_H^{model}(\mathbf{r}, n^{hom}(\mathbf{r}))$$

Now approximate, e.g.  $\frac{1}{|\mathbf{r}-\mathbf{r}'|} \rightarrow c$

*In original expression:*

$$v_H(\mathbf{r}) \approx N*c$$

*In connector:*  $n^{hom}(\mathbf{r}, [n]) = \frac{1}{4\pi R^3/3} \int d\mathbf{r}' n(\mathbf{r}') = \bar{n}$  MDA

Correct long-range behaviour,  $c$  cancels!!!

$$v_H(\mathbf{r}) \approx \bar{n} \int_R d\mathbf{r}' \frac{1}{|\mathbf{r}-\mathbf{r}'|}$$

## → Connector Theory: Example

*Target:* Hartree potential of finite system. *Model:* jellium sphere.

$$v_H(\mathbf{r}, [n]) = \int d\mathbf{r}' \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \stackrel{!}{=} n^{hom} \int_R d\mathbf{r}' \frac{1}{|\mathbf{r} - \mathbf{r}'|}$$

**Errors due to approximations cancel in connector**

**Model system tabulated and used in simple way**

$$v_H(\mathbf{r}, [n]) = v_H^{model}(\mathbf{r}, n^{hom}(\mathbf{r}))$$

Now approximate, e.g.  $\frac{1}{|\mathbf{r}-\mathbf{r}'|} \rightarrow c$

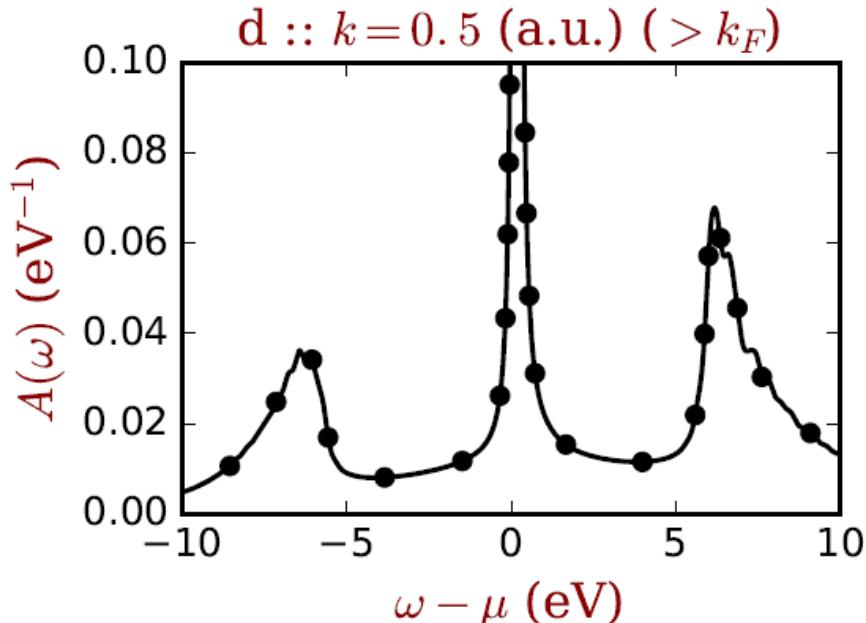
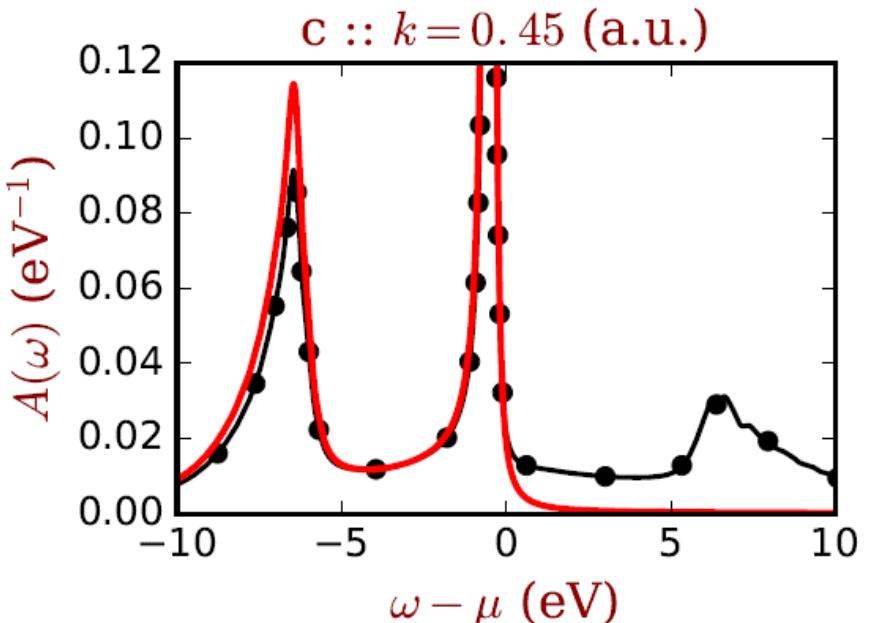
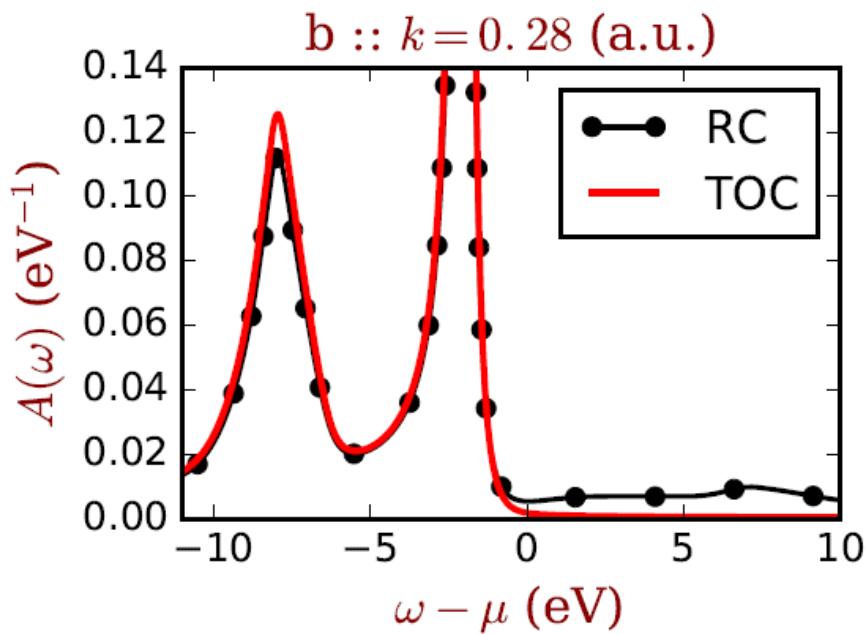
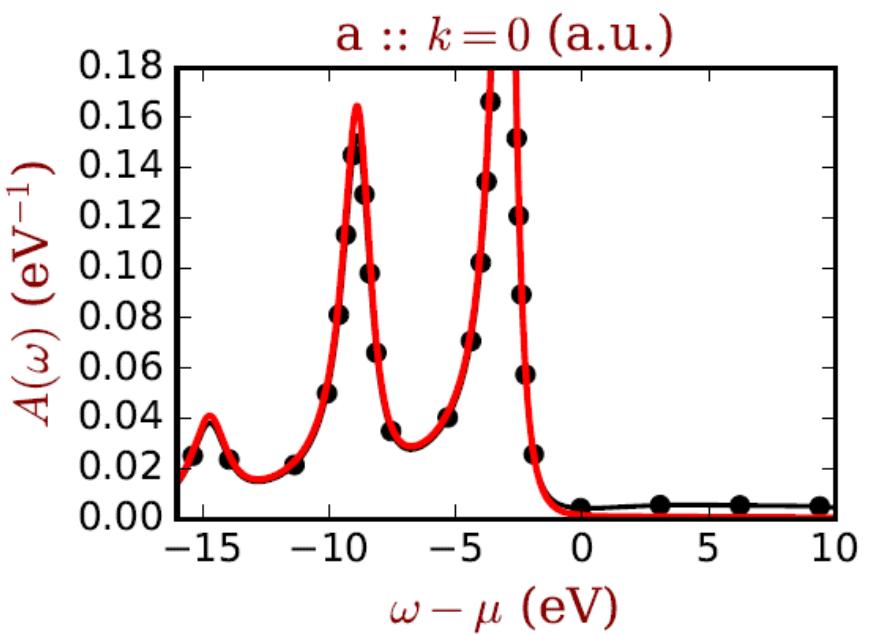
*In original expression:*

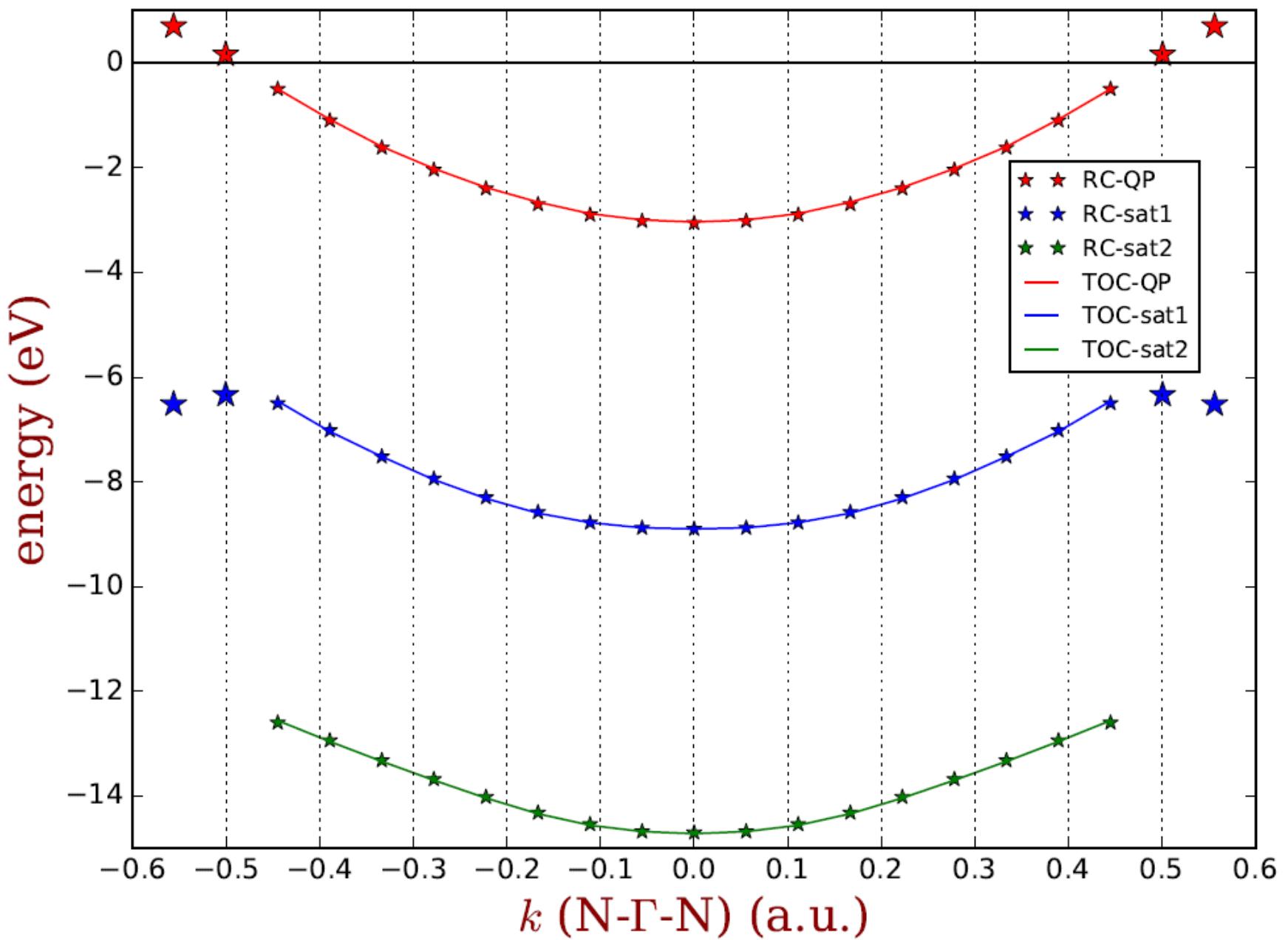
$$v_H(\mathbf{r}) \approx N/c$$

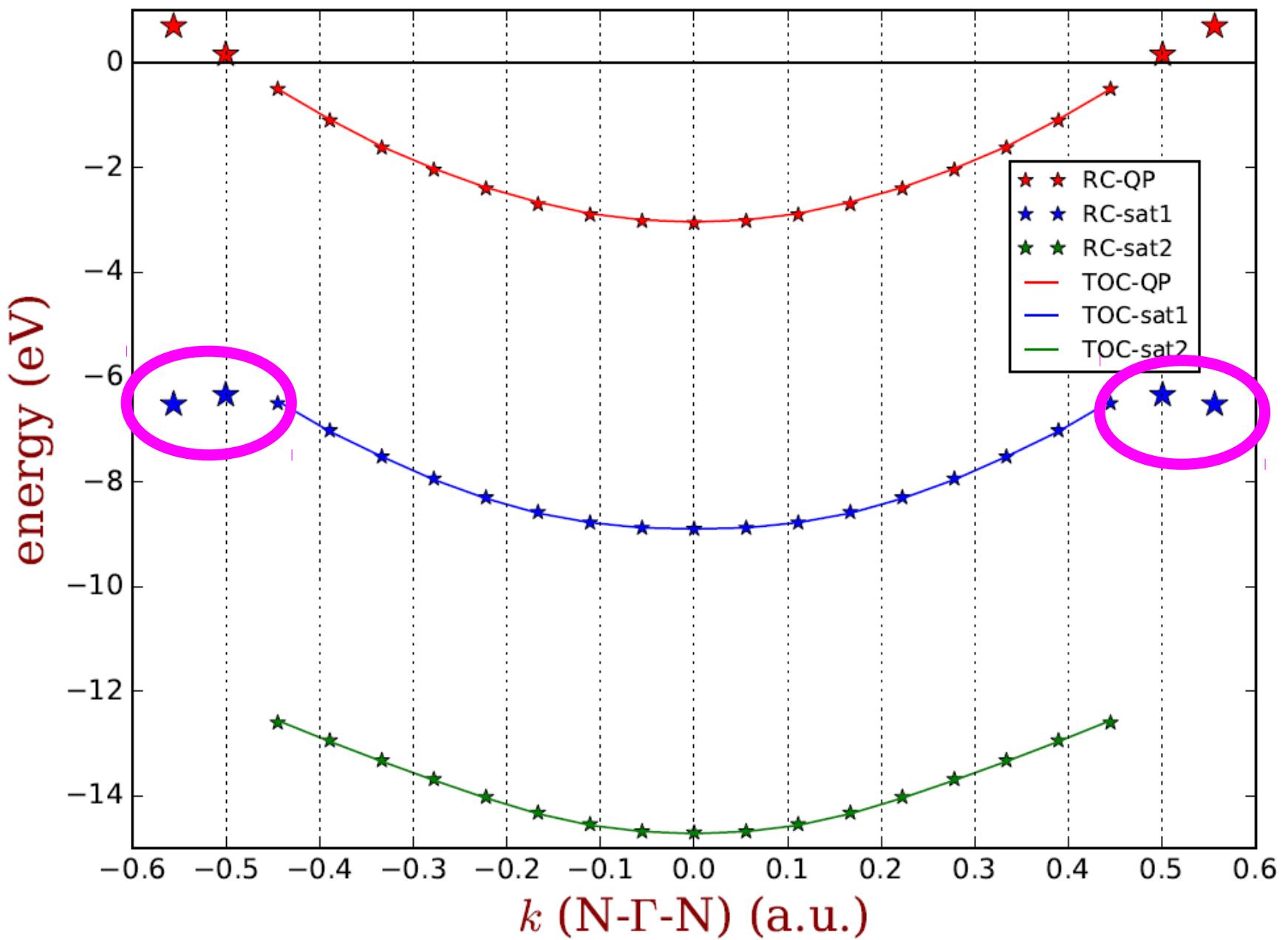
*In connector:*  $n^{hom}(\mathbf{r}, [n]) = \frac{1}{4\pi R^3/3} \int d\mathbf{r}' n(\mathbf{r}') = \bar{n}$

Correct long-range behaviour,  $c$  cancels!!!

$$v_H(\mathbf{r}) \approx \bar{n} \int_R d\mathbf{r}' \frac{1}{|\mathbf{r}-\mathbf{r}'|}$$

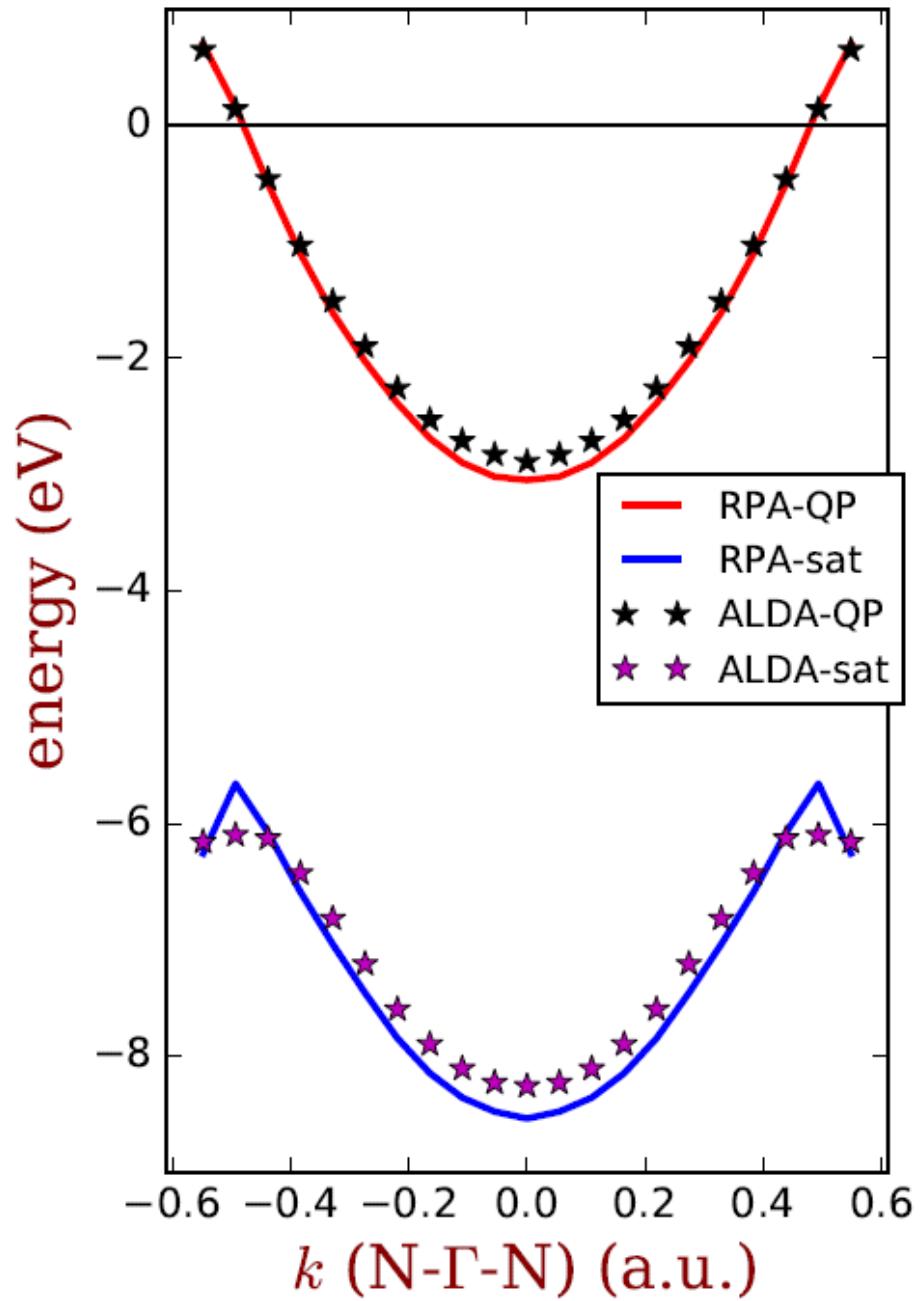






## Approximation for screening

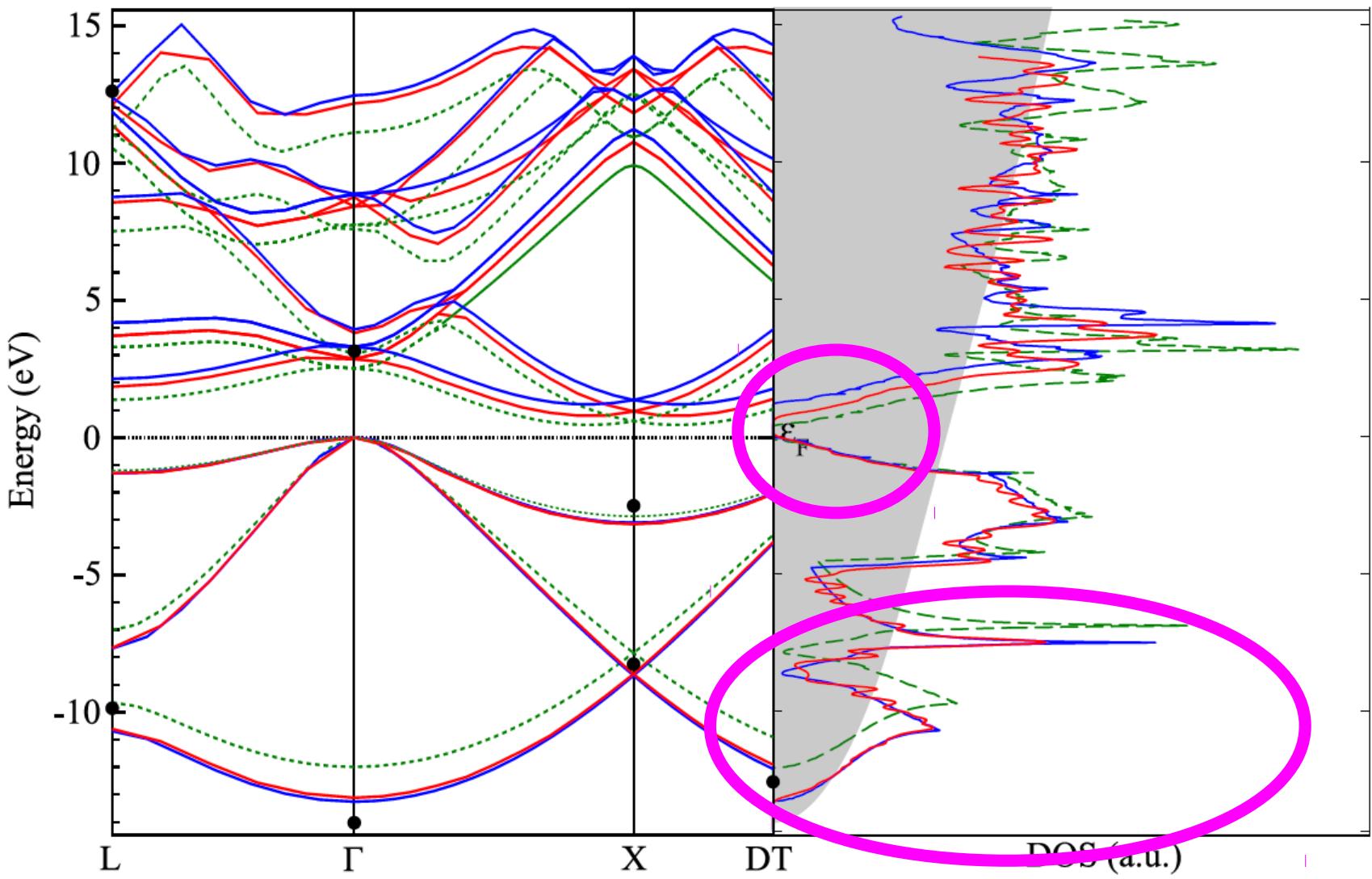
c :: band  $\Gamma$ -N



# Silicon

— LDA  
— HSE06

— dynLDA



→ As a model system, we stay with the HEG

$v_{xc}$  in the HEG from QMC (Ceperley and Alder)

But  $f_{xc}$  ?

Martin Panholzer, following

H. M. Boehm, R. Holler, E. Krotscheck, and M. Panholzer,  
Phys. Rev. B 82, 224505 (2010)

→ Calculate  $\chi$  in the HEG:

- action with Jastrow wavefunction
- linear response
- selected number of excitations
- $S(q)$  from QMC

→ Calculate  $f_{xc}$  in the HEG by inverting  $\chi = \chi_0 + \chi_{\perp} [v + f_{xc}] \chi$

$$|\Psi_0\rangle \equiv F|\Phi_0\rangle = \exp \left\{ \frac{1}{2} \left( \sum_i u^{(1)}(\mathbf{r}_i) + \sum_{i < j} u^{(2)}(\mathbf{r}_i, \mathbf{r}_j) + \dots \right) \right\} |\Phi_0\rangle$$

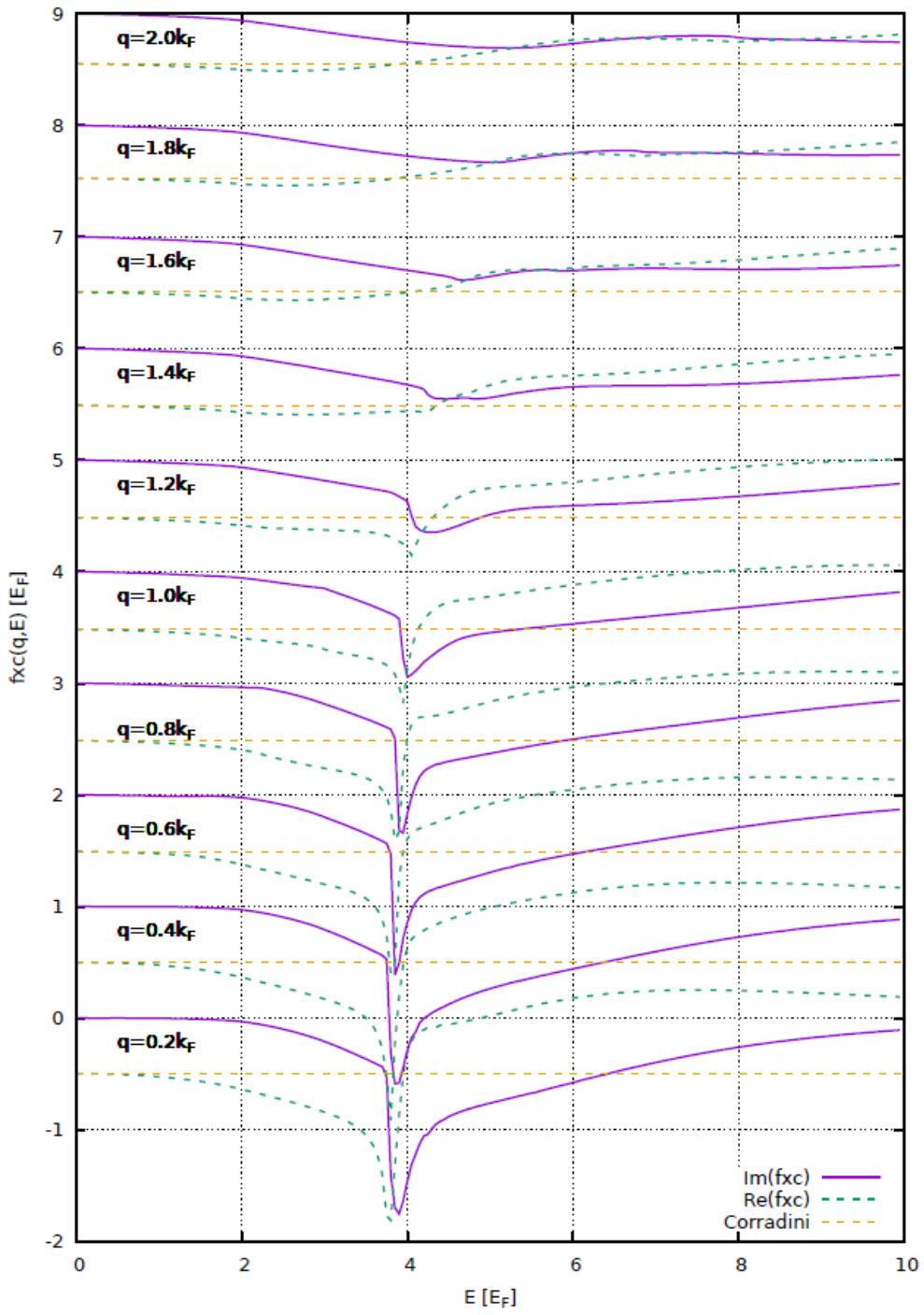
$$|\Psi_t\rangle = \frac{e^{-iE_0 t/\hbar}}{\sqrt{\mathcal{N}}} F e^{\delta U(t)} |\Phi_0\rangle, \quad \mathcal{N} \equiv \langle \Psi_t | \Psi_t \rangle$$

$$\delta U(t) = \sum_{ph} \delta u_{ph}^{(1)}(t) a_p^\dagger a_h + \frac{1}{2} \sum_{pp'hh'} \delta u_{pp'hh'}^{(2)}(t) a_p^\dagger a_{p'}^\dagger a_{h'} a_h + \dots$$

Equations of motion for correlation amplitudes

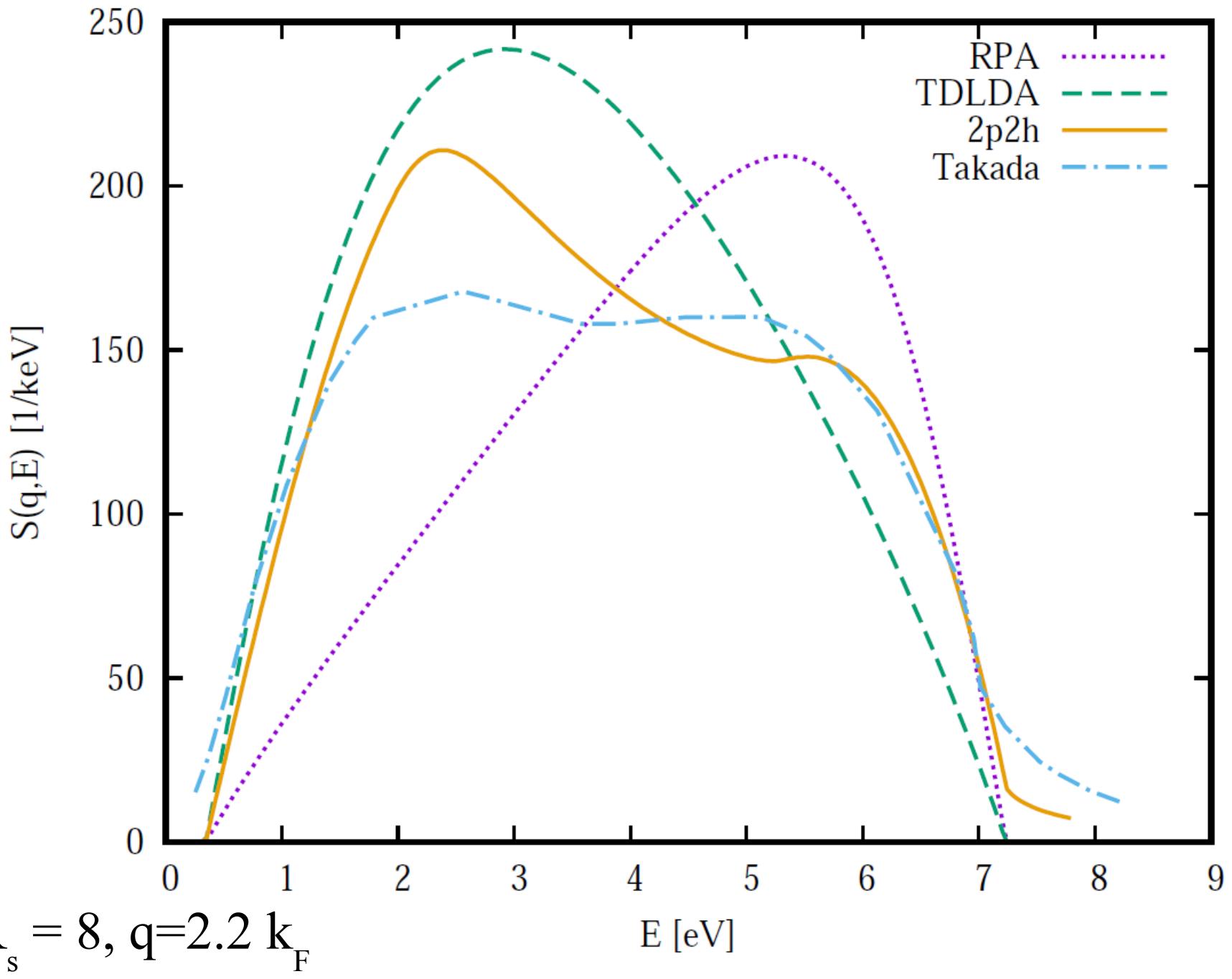
$S(q)$  enters result; taken from QMC

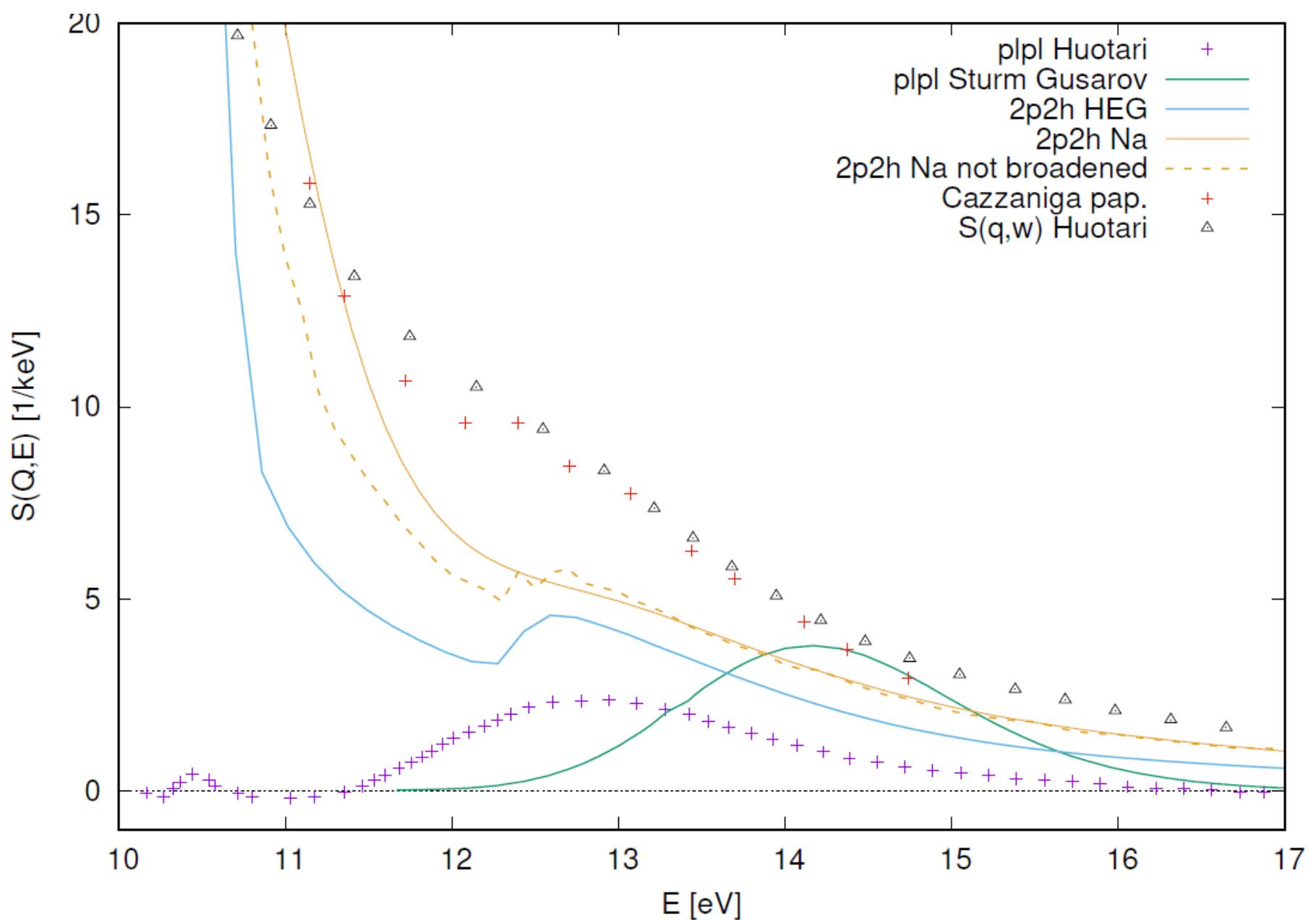
# HEG $f_{xc}$



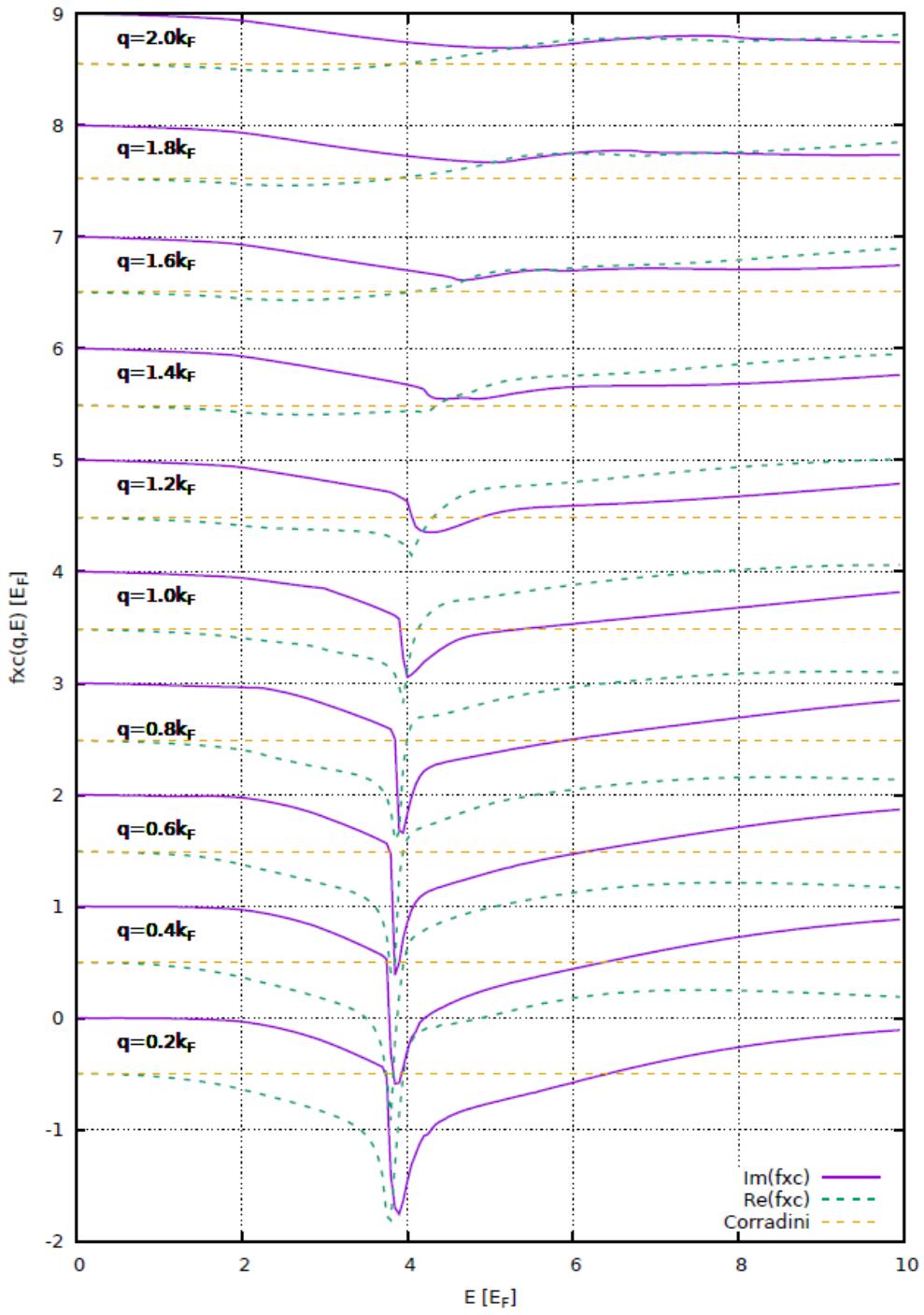
Static: M. Corradini, R. Del Sole,  
G. Onida, and M. Palummo,  
Phys. Rev. B 57, 14569 (1998).

Dynamic: Martin Panholzer et al.





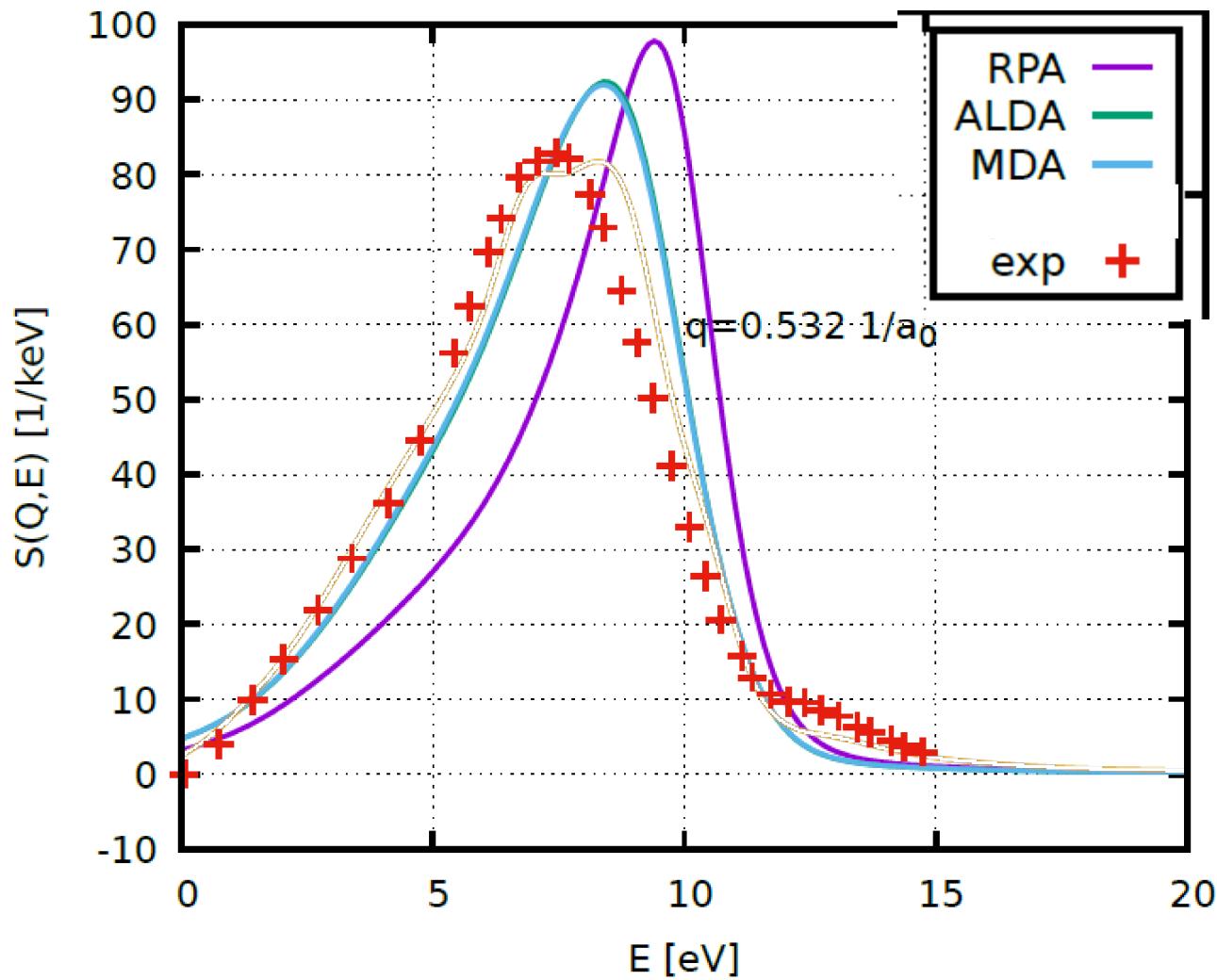
# HEG $f_{xc}$



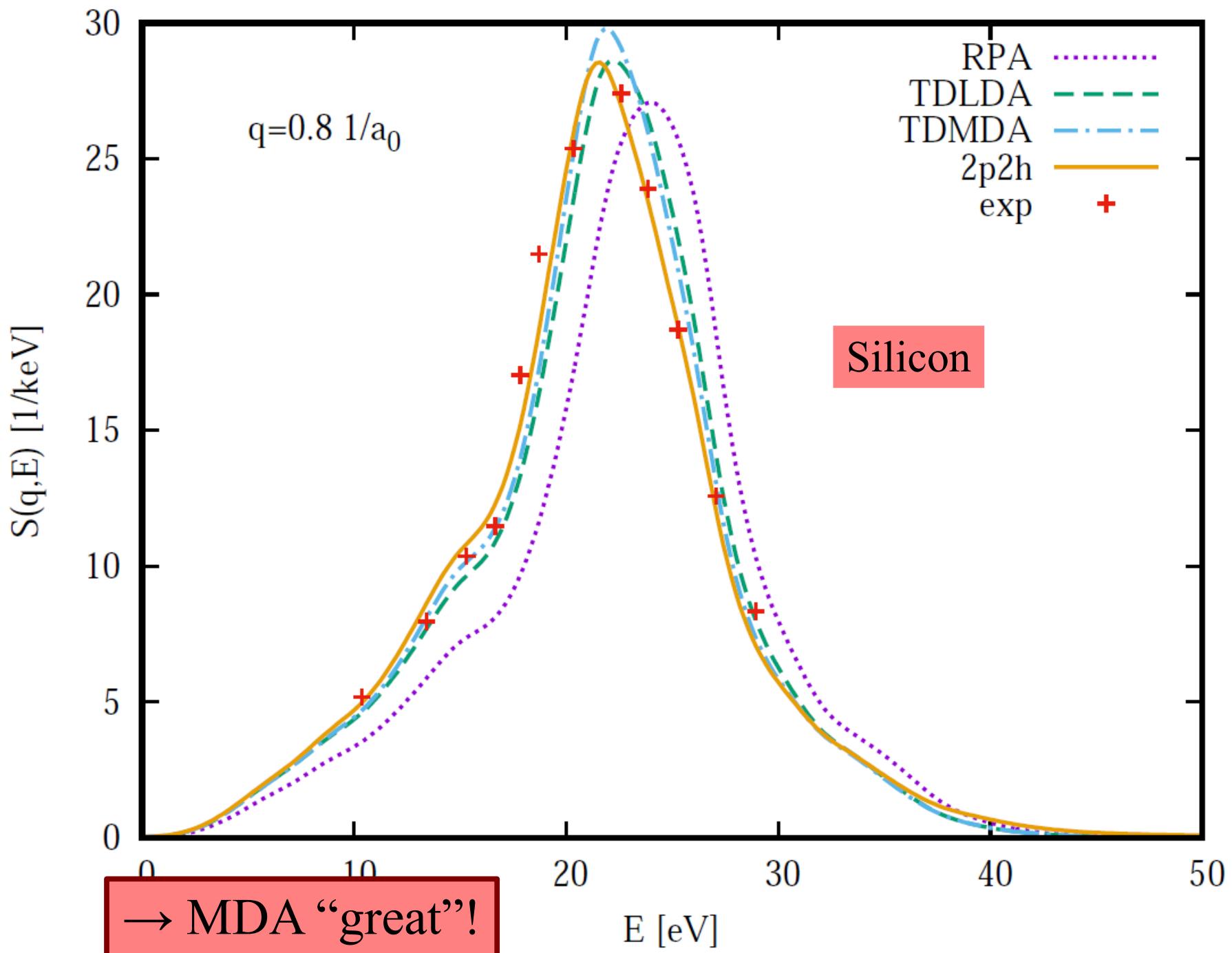
Static: M. Corradini, R. Del Sole,  
G. Onida, and M. Palummo,  
Phys. Rev. B 57, 14569 (1998).

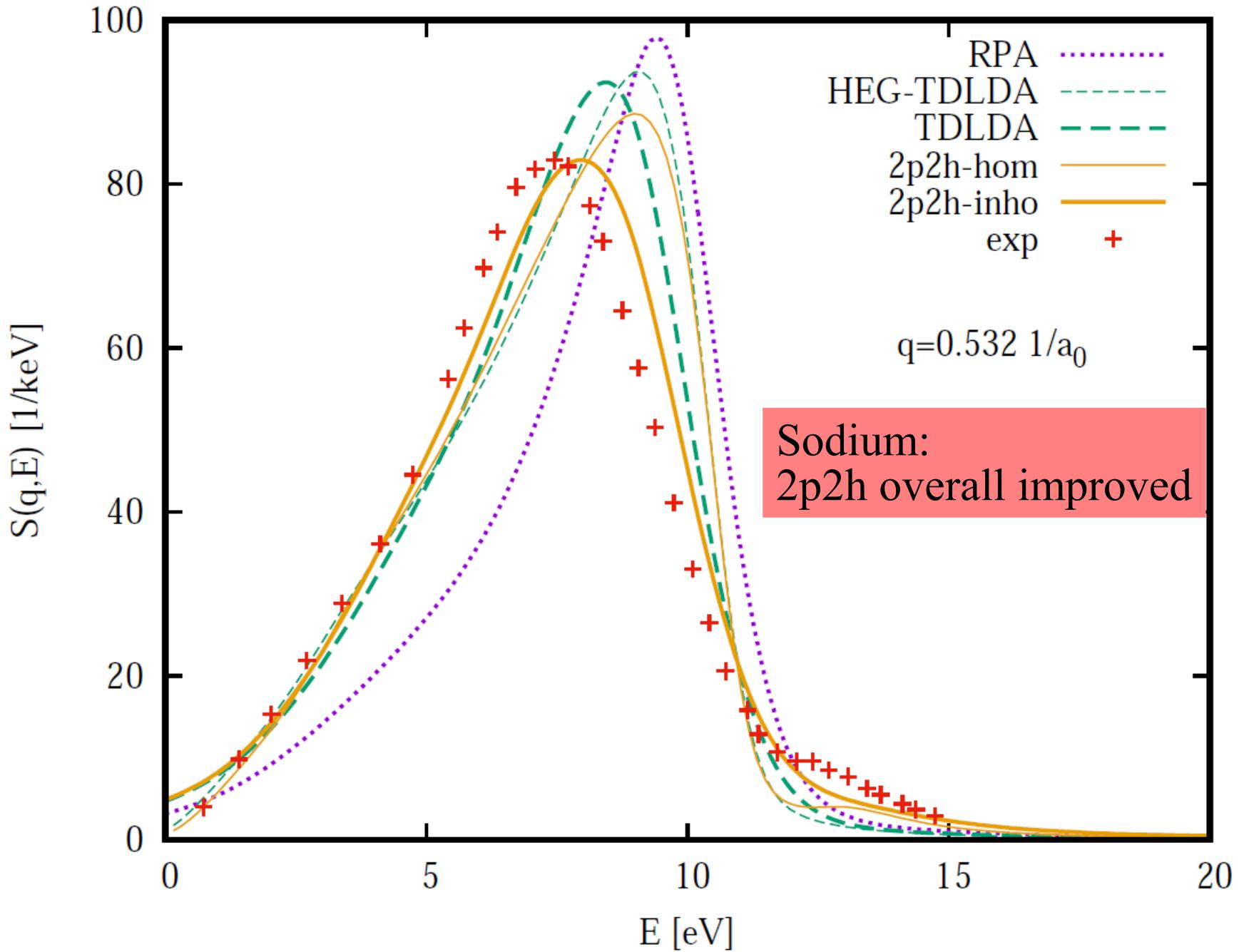
Dynamic: Martin Panholzer et al.

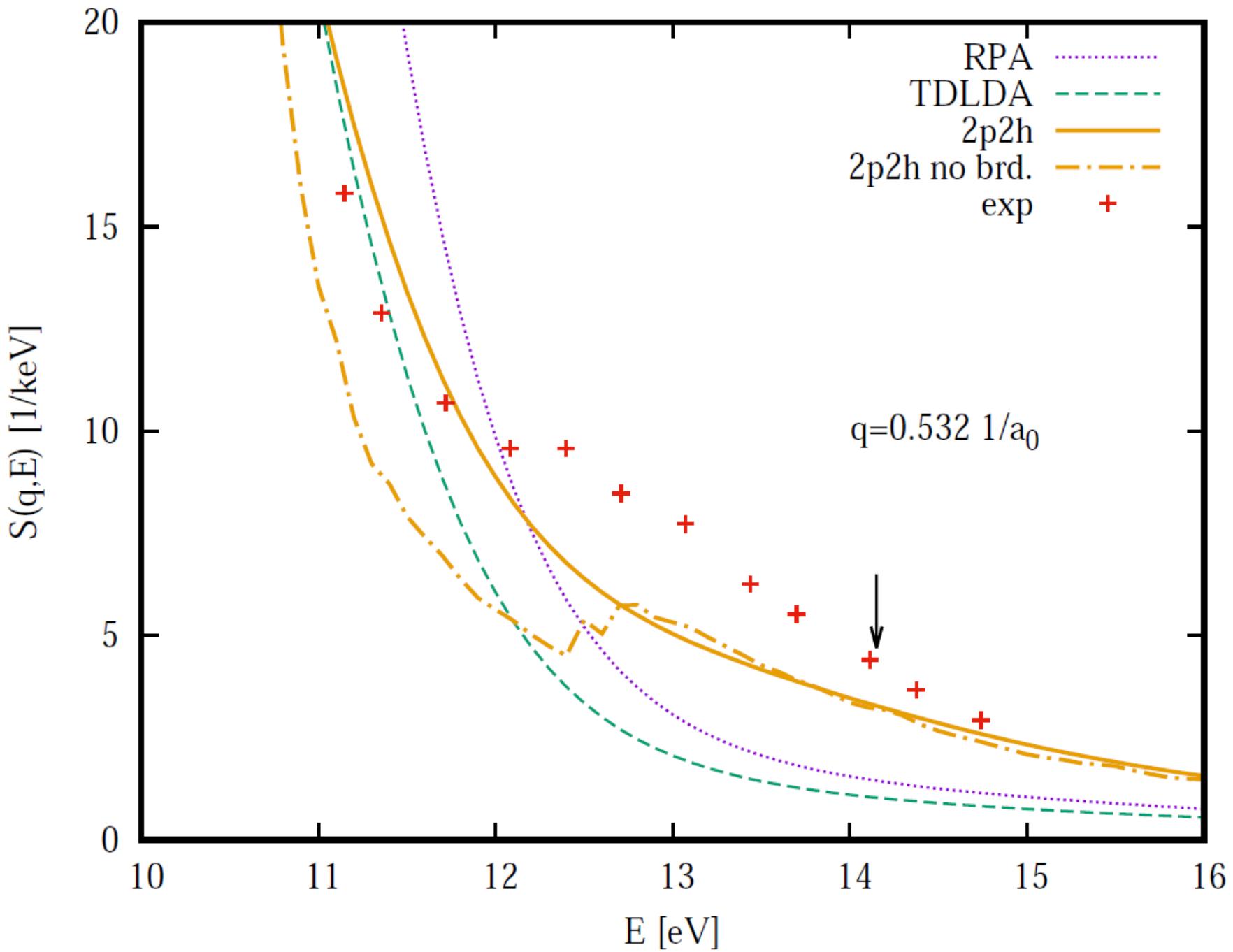
Connector for  $f_{xc}(r,t;r',t')$ :  
“mean density approximation”



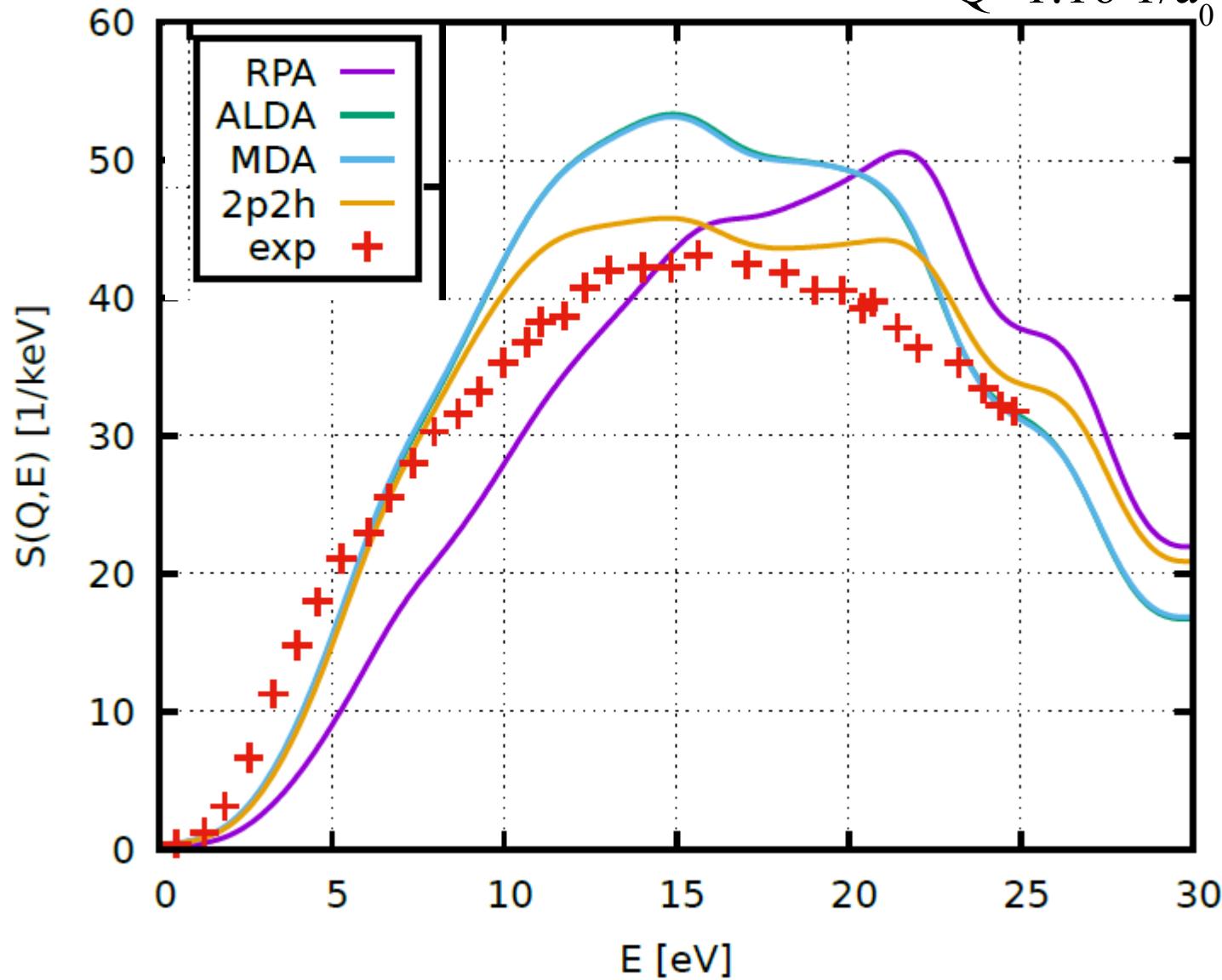
→ MDA “great”!



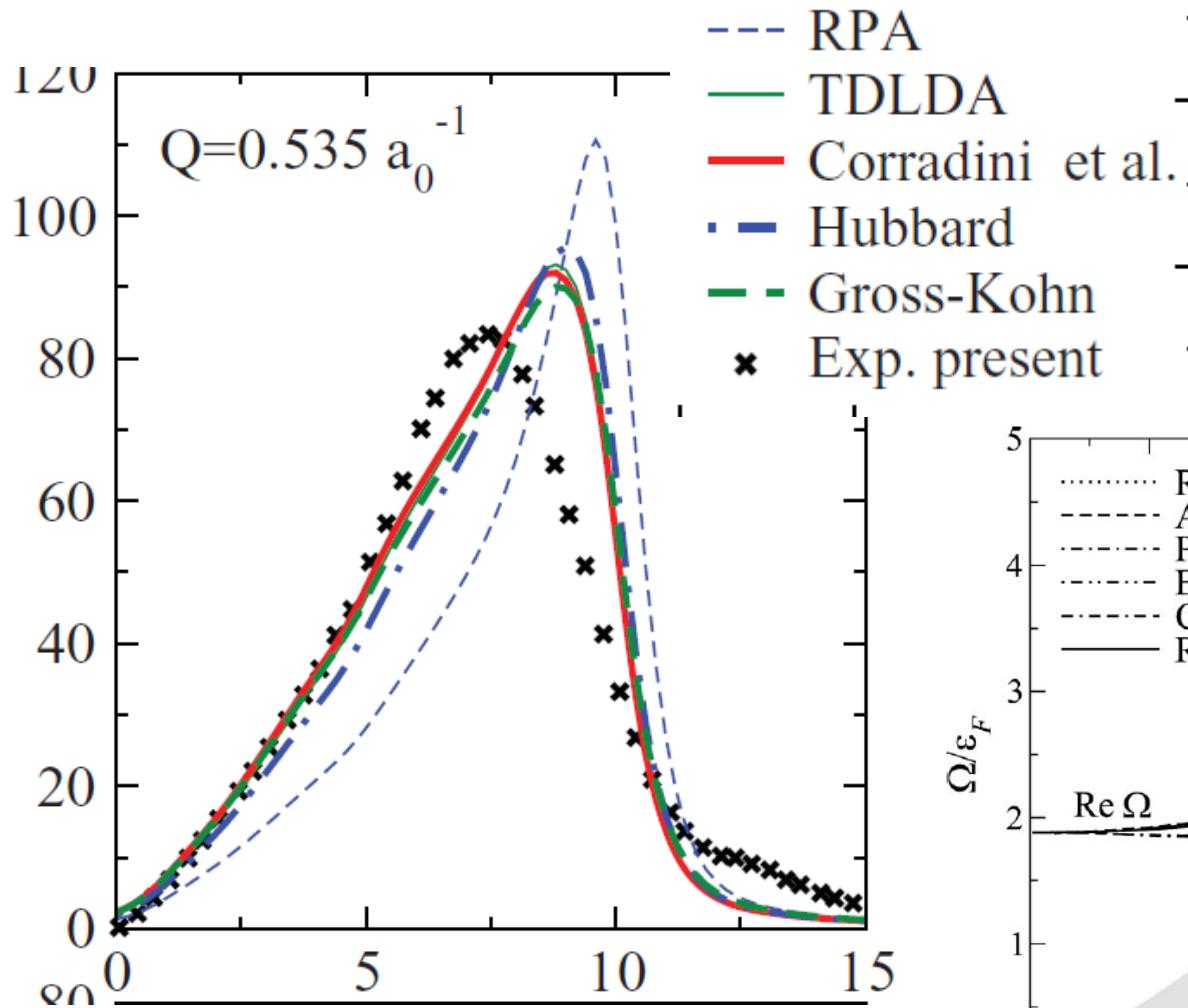




$Q=1.16 \frac{1}{a_0}$

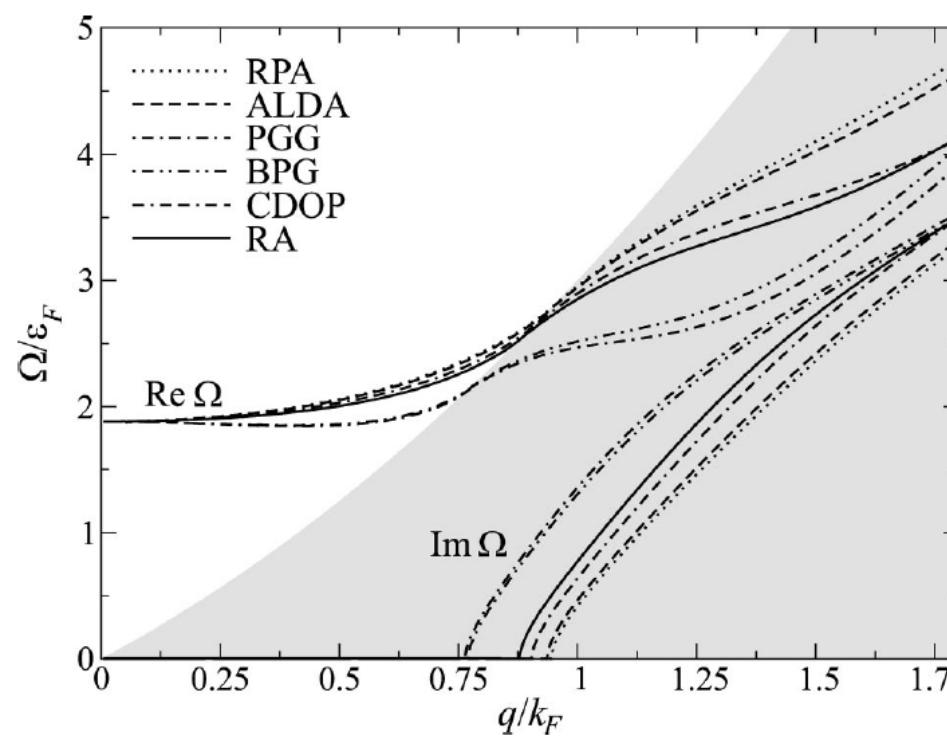


## Efforts to improve plasmon spectra



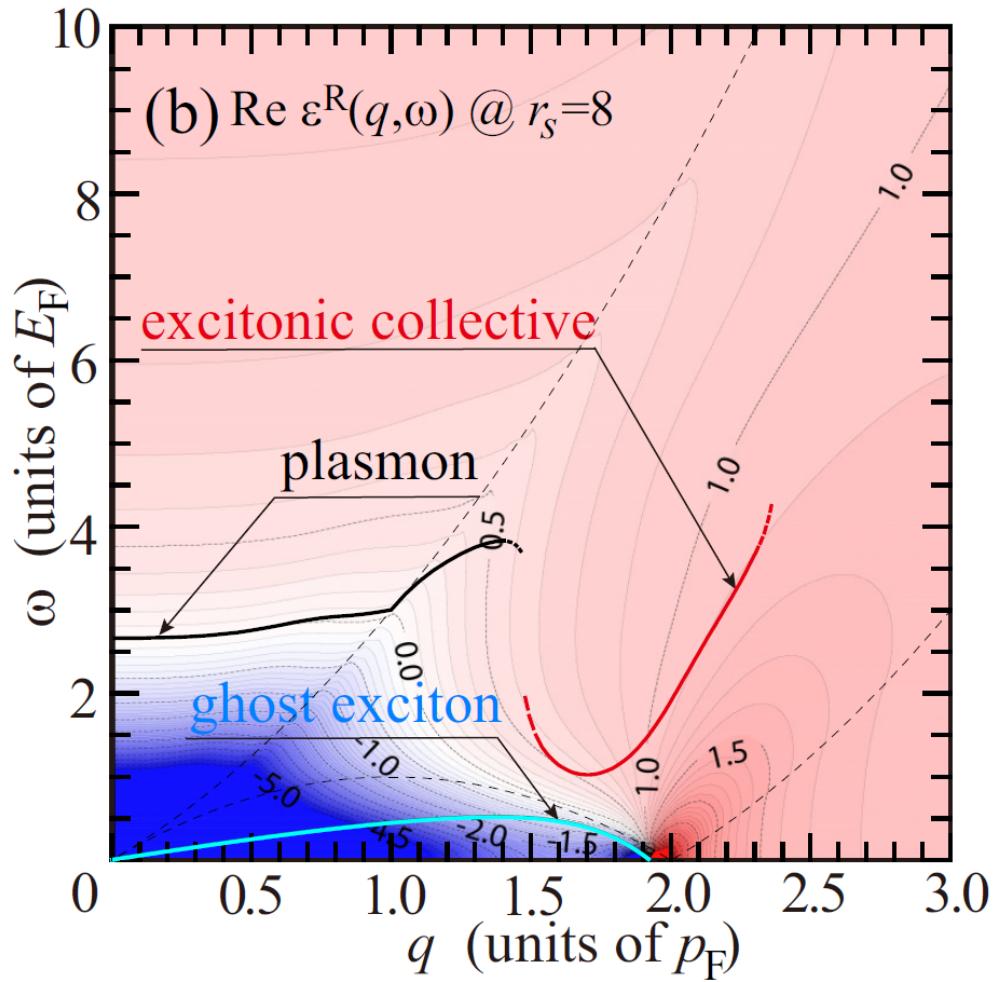
Cazzaniga et al., PRB 84, 075109 (2011)

Sodium



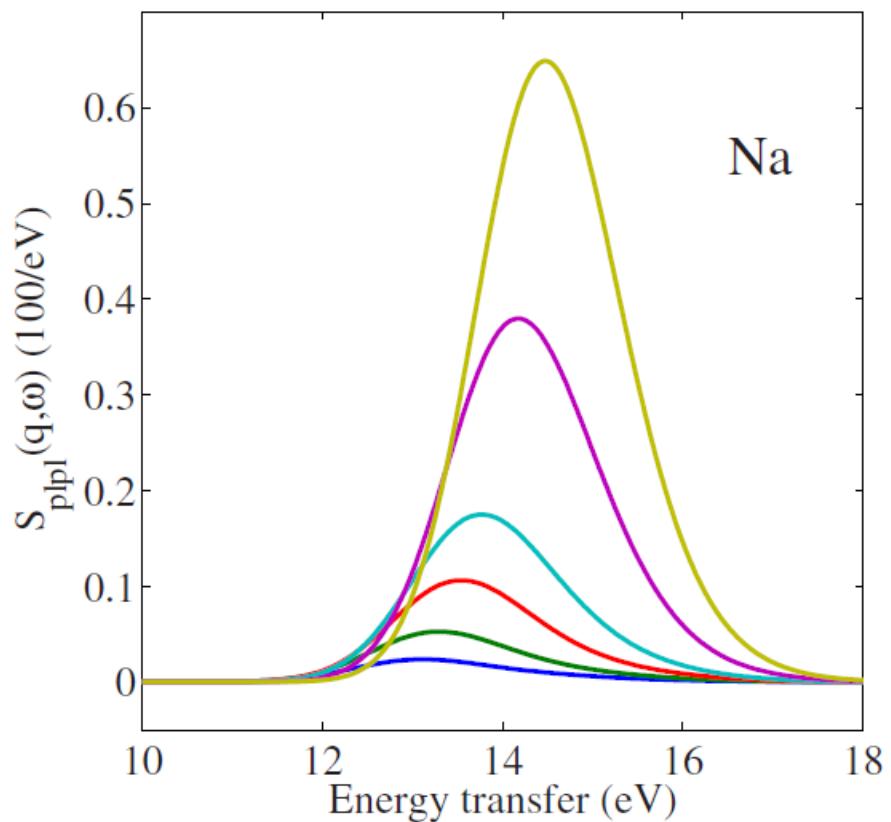
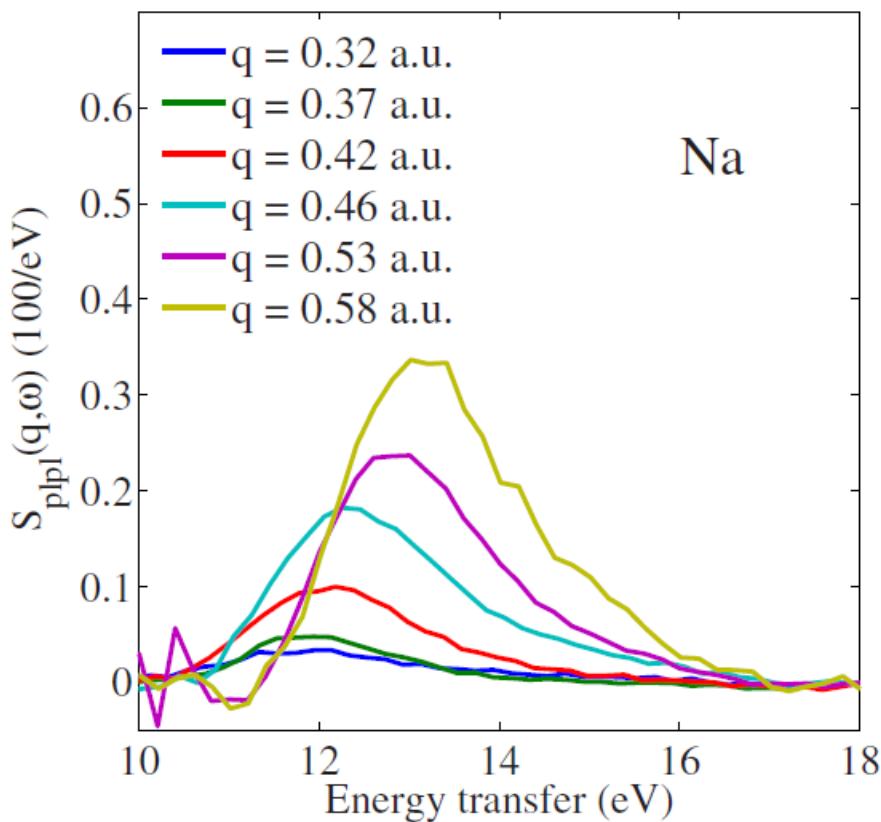
Tatarczyk et al., PRB 63, 235106

## Modified Richardson-Ashcroft kernel: new spectral features



# Diagrammatic derivation of the double plasmon

→ Compares qualitatively, not quantitatively

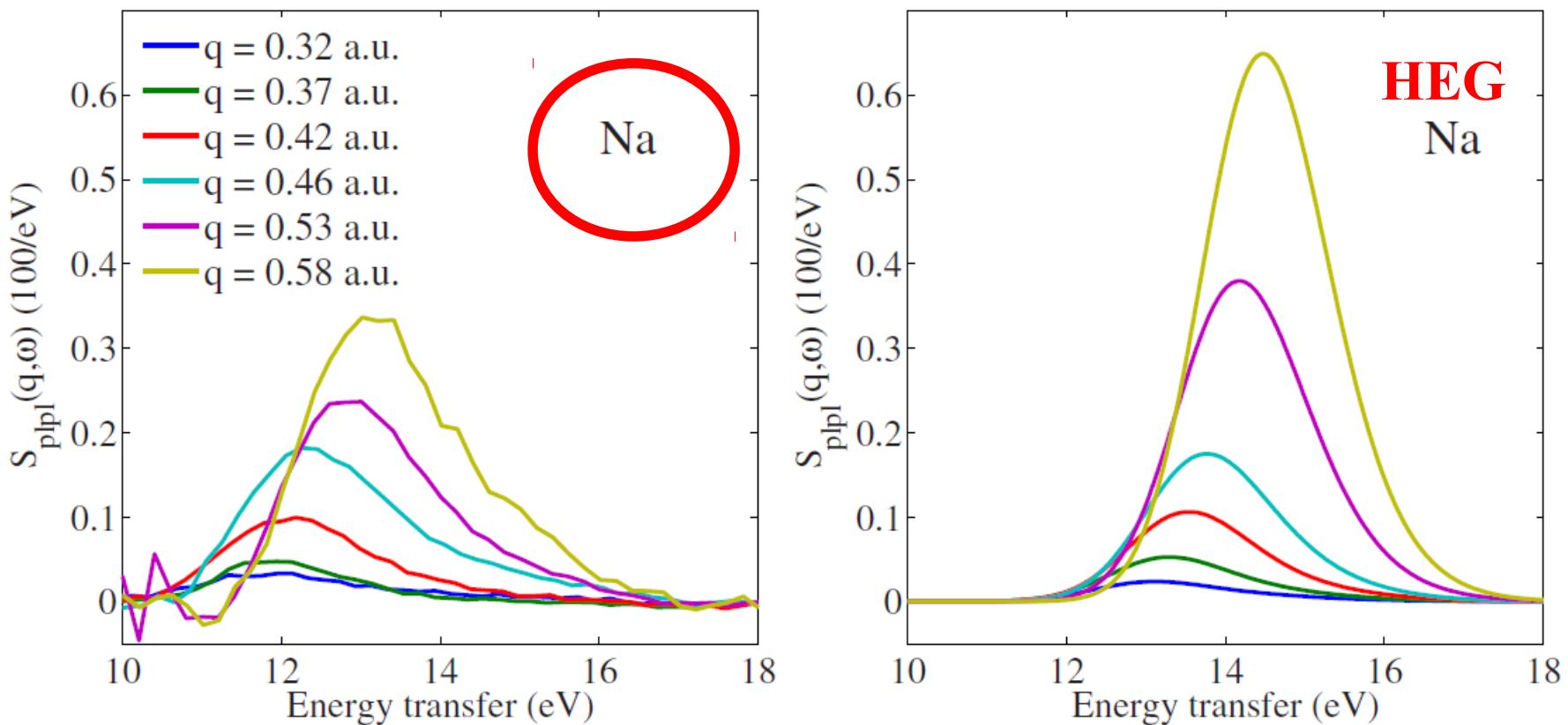


S. Huotari et al., PRB 77, 195125 2008

Prediction: K. Sturm and A. Gusarov, Phys. Rev. B 62, 16474 2000.

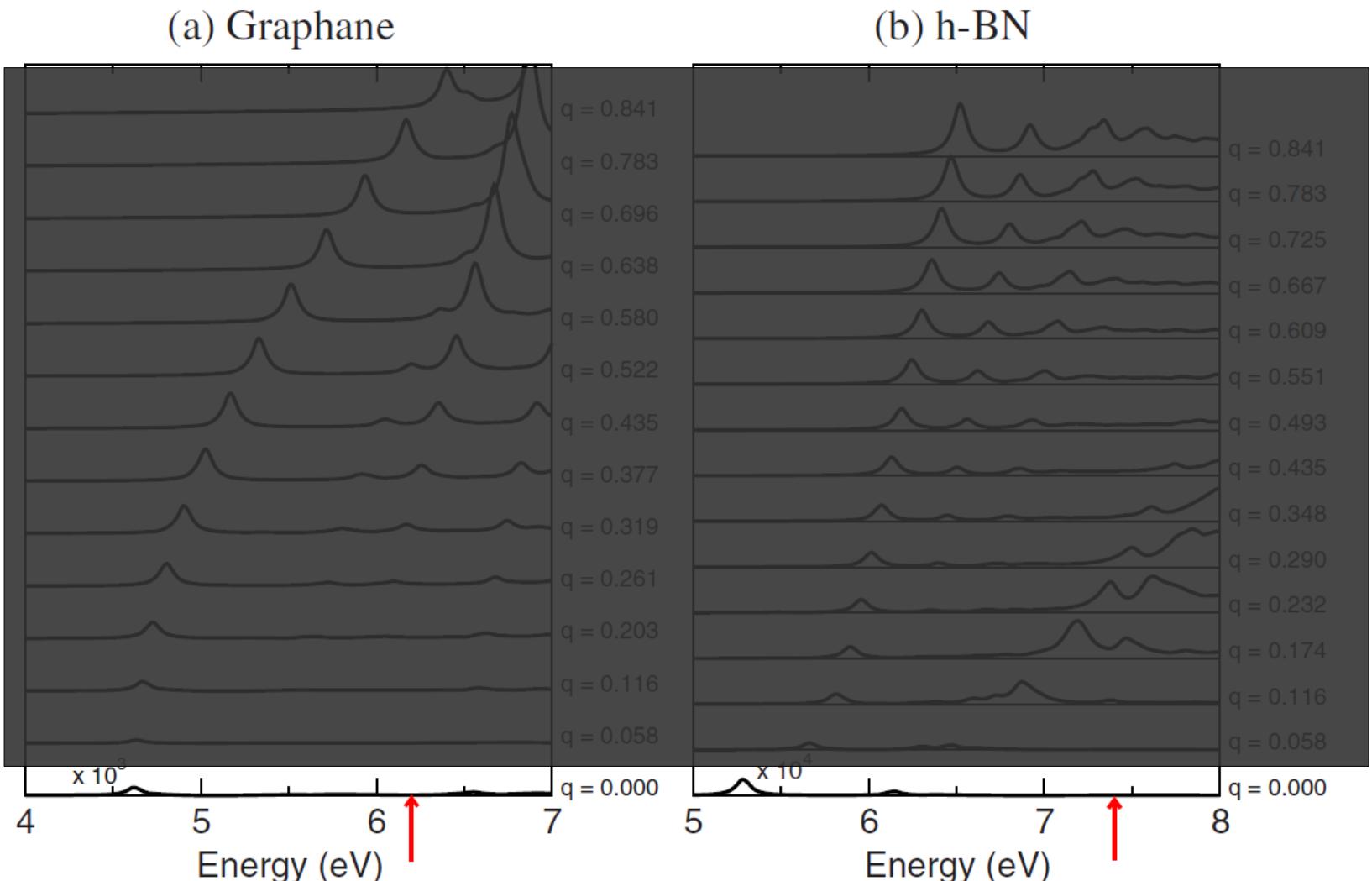
# Diagrammatic derivation of the double plasmon

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S. Huotari et al., PRB 77, 195125 2008

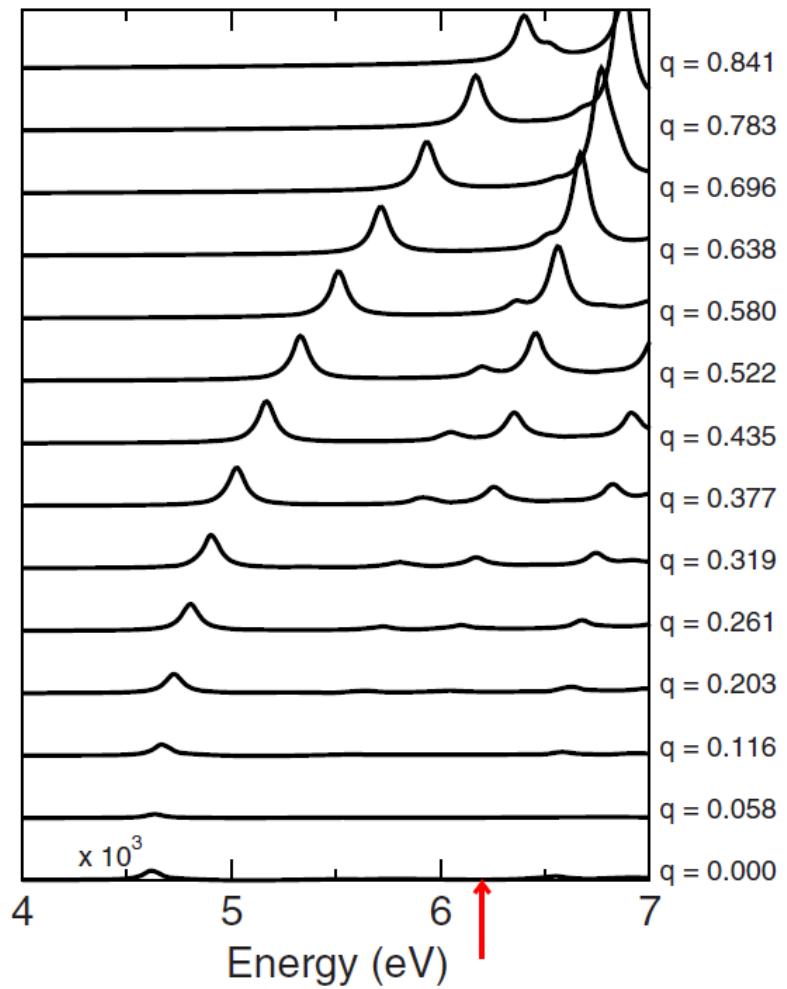
Prediction: K. Sturm and A. Gusarov, Phys. Rev. B 62, 16474 2000.



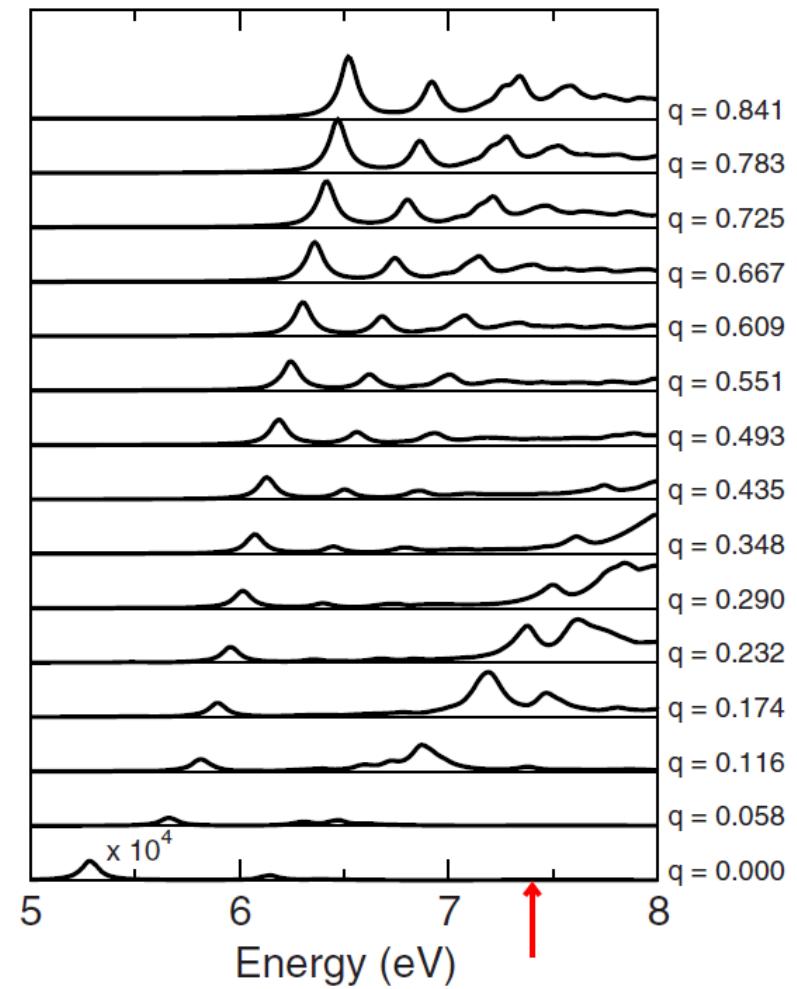
P. Cudazzo et al., PRL 116, 066803 (2016)

W. A. Caliebe et al. Phys. Rev. Lett., 2000; A. Marini, R. Del Sole, and A. Rubio, Phys. Rev. Lett., 2003  
 M. Gatti and F. Sottile, Phys. Rev. B 88, 155113 (2013)

(a) Graphene



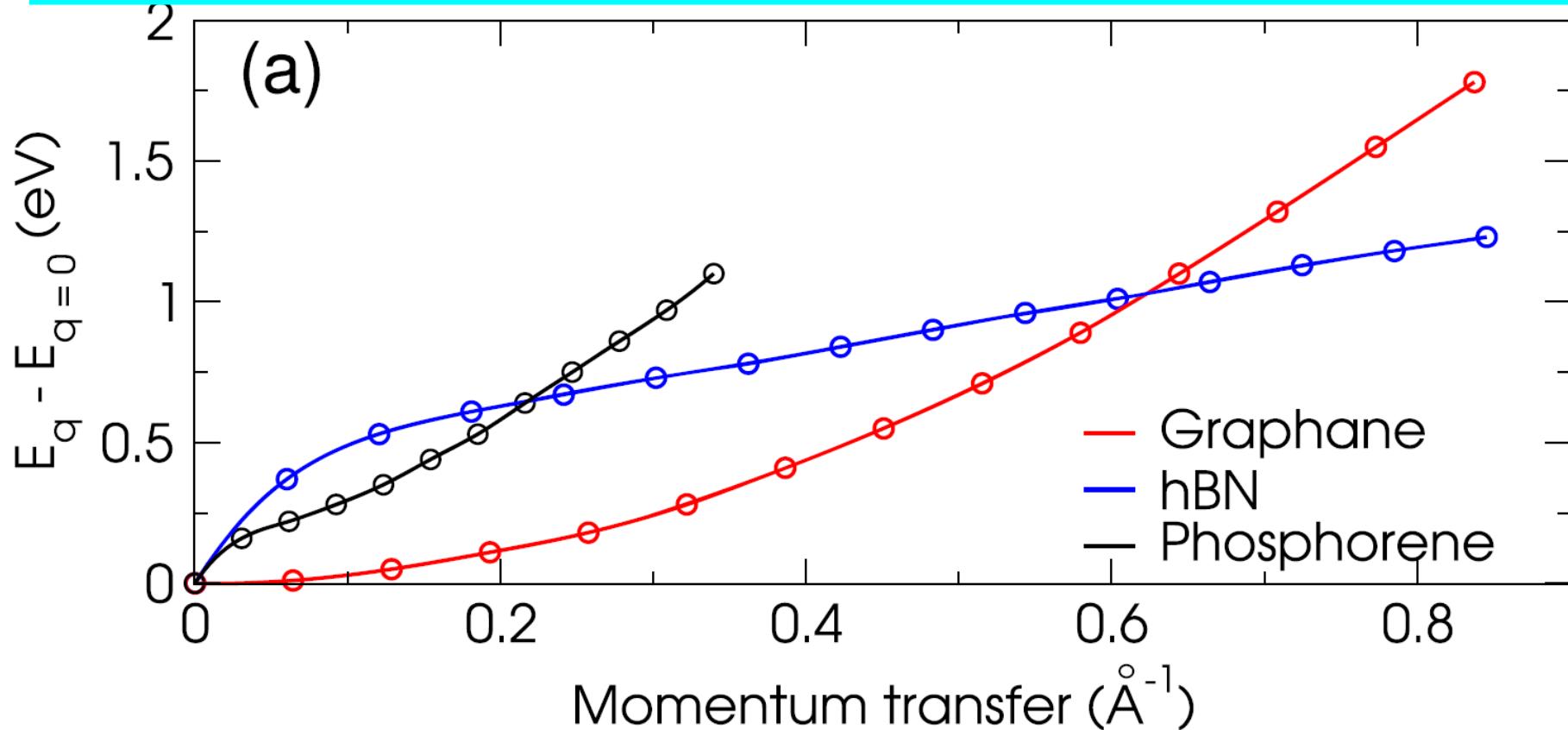
(b) h-BN



P. Cudazzo et al., PRL 116, 066803 (2016)

W. A. Caliebe et al. Phys. Rev. Lett., 2000; A. Marini, R. Del Sole, and A. Rubio, Phys. Rev. Lett., 2003  
M. Gatti and F. Sottile, Phys. Rev. B 88, 155113 (2013)

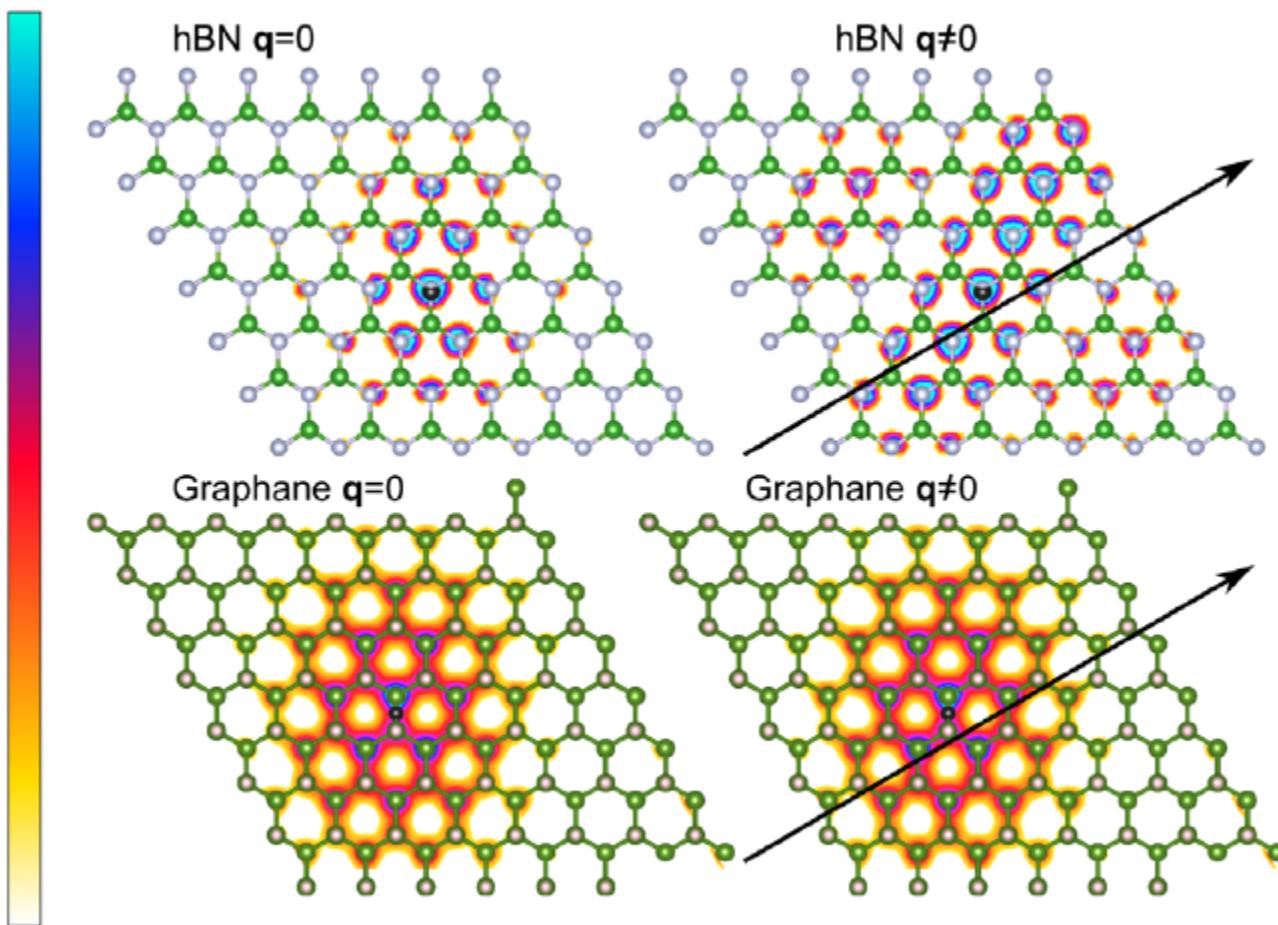
# How to characterize an exciton in 2D? Beyond q=0 !



Binding energy:

graphane	1.6 eV
h-BN	2.1 eV
Phosphorene	0.6 eV

P. Cudazzo et al., PRL 116, 066803 (2016)

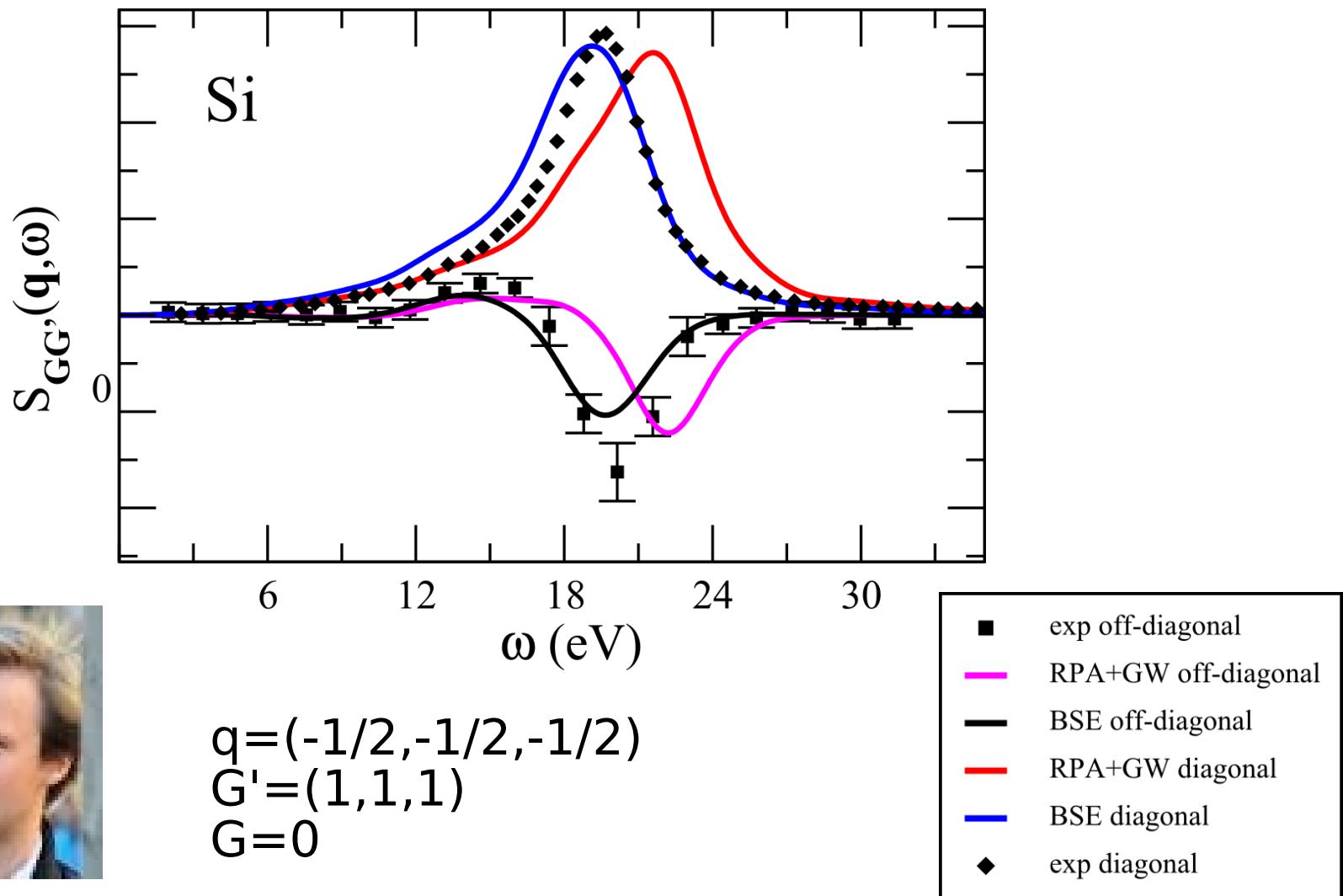


$$V_{\text{tot}}(r, \omega) = \int dr' \epsilon^{-1}(r, r', \omega) V_{\text{ext}}(r', \omega)$$

$$\epsilon^{-1}(r, r', \omega) \rightarrow \boxed{\epsilon^{-1}_{GG'}(q, \omega)}$$

Full matrix!

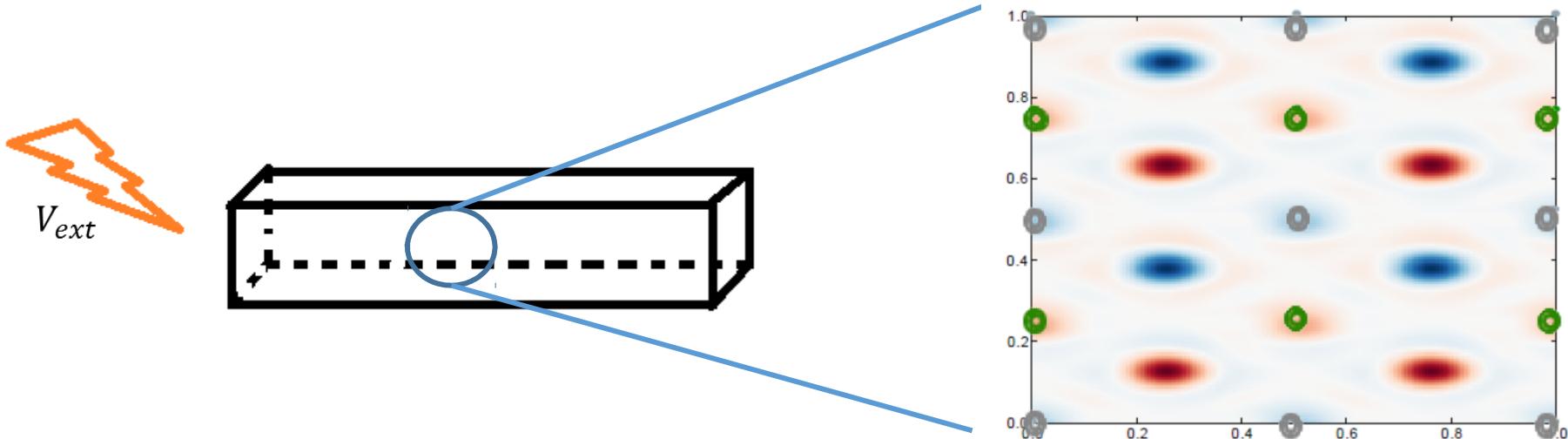
# Macro/micro-scopic perturbation → macro/micro-scopic response



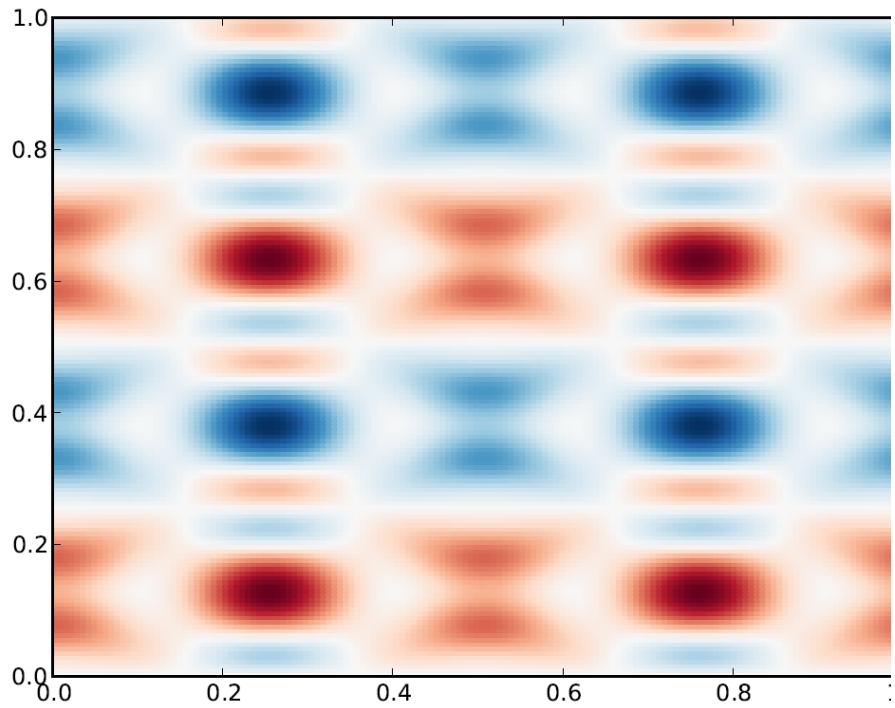
Igor Reshetnyak

Dia: H.C. Weissker et al. Phys. Rev. B (2010)  
Off-dia: W. Schülke and A. Kaprolat Phys. Rev. Lett. (1991)

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

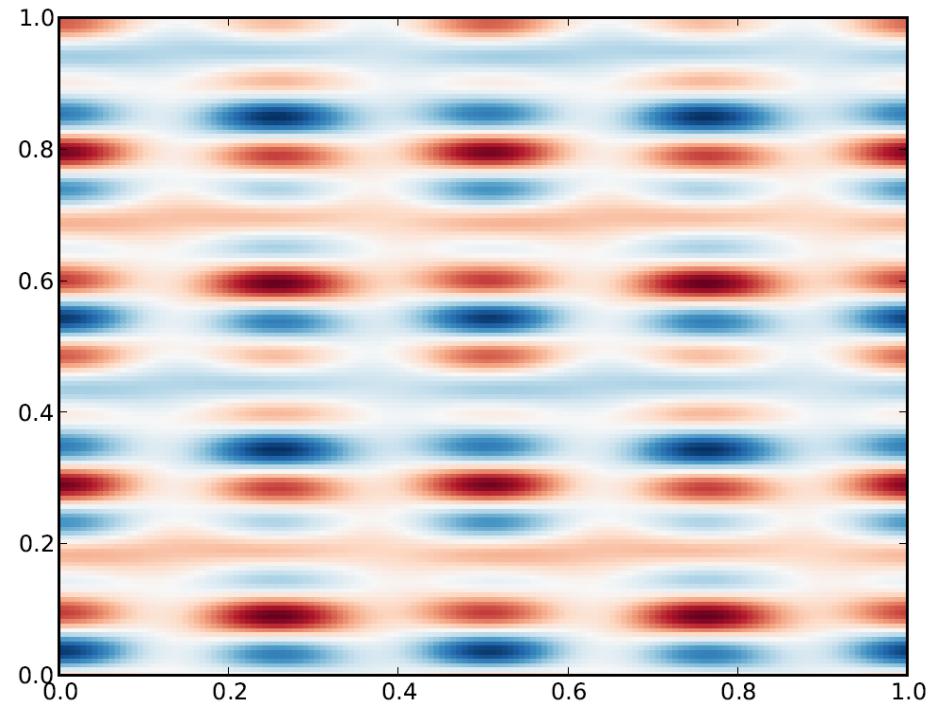


Ralf Hambach, Giulia Pegolotti, Claudia Roedl, Igor Reshetnyak



RPA

At 14.1 eV



BSE

*The whole matrix → follow excitations in real space and time*

# Cumulant expansions

Similar for 2-body Green's function (absorption, loss,...):

J. S. Zhou et al., JCP 143, 184109 (2015) → P. Cudazzo & L. Reining (2018)

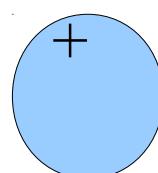
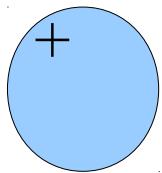
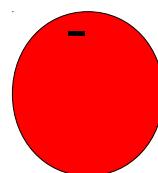
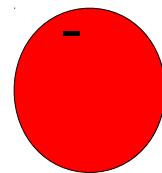
$$P_{\lambda\lambda}^<(\mathbf{q}, t_{13}) = e^{-iE_\lambda \mathbf{q}(t_3 - t_1) + C_{\lambda\mathbf{q}}(t_{13})} \quad \text{G} \rightarrow \text{P}$$

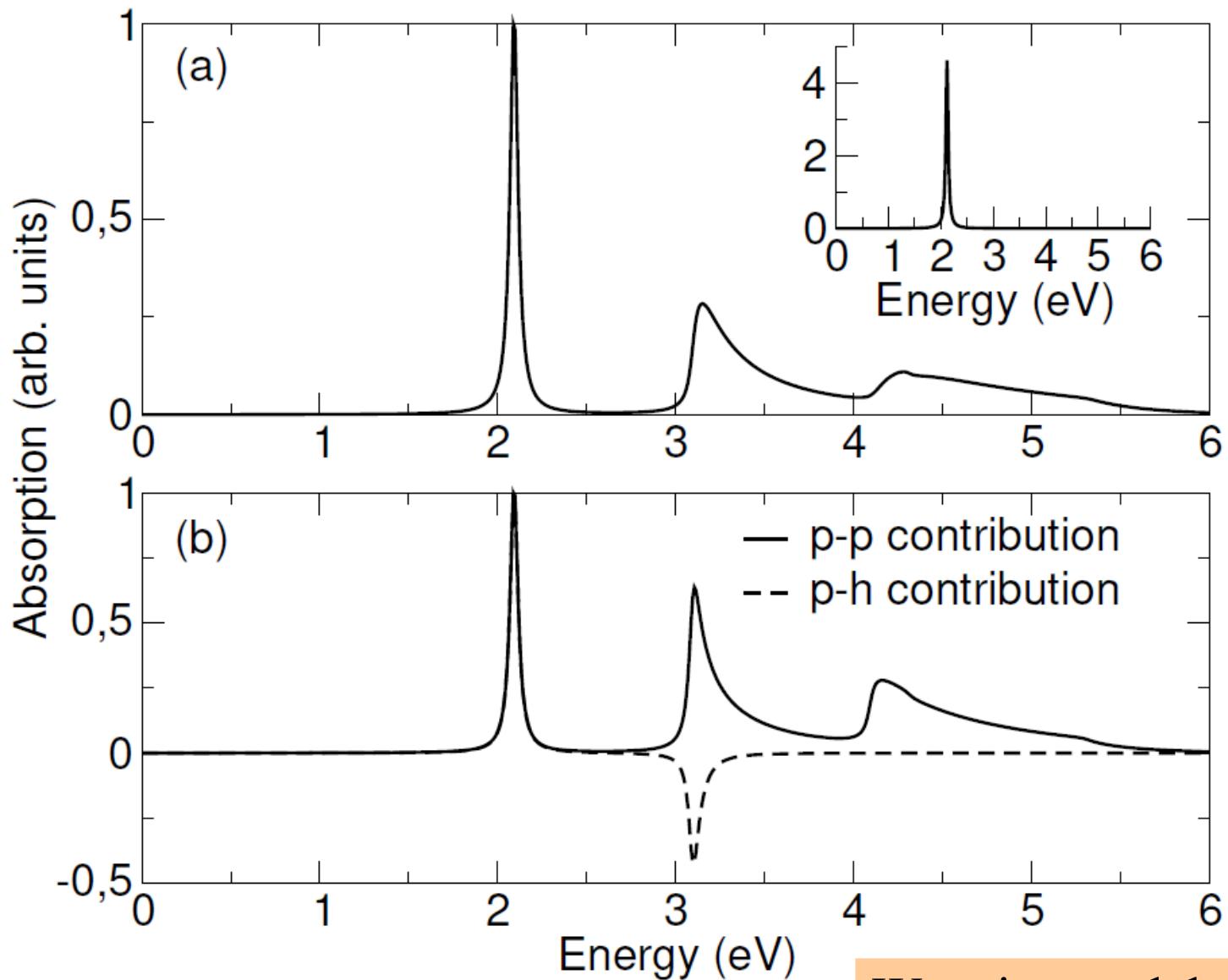
$$C_{\lambda\mathbf{q}}(t_{13}) = \int_{t_1}^{t_3} dt_{1'} \int_{t_{1'}}^{t_3} dt_{3'} \Pi_{\lambda\lambda}(\mathbf{q}, t_{1'3'}) e^{iE_\lambda \mathbf{q}(t_{3'} - t_{1'})} \quad \Sigma \rightarrow \Pi$$

$$\Pi_{\lambda\lambda'}(\mathbf{q}, t_{13}) = \sum_{\alpha\mathbf{q}'} \mathcal{W}_{\lambda\mathbf{q}\alpha\mathbf{q}'\alpha\mathbf{q}'\lambda'\mathbf{q}}(t_{13}) \bar{P}_{\alpha\alpha}(\mathbf{q}', t_{13}) \quad \text{G}^{\text{QP}} \rightarrow \overline{\text{P}}$$

$$\text{W} \rightarrow \mathcal{W}$$

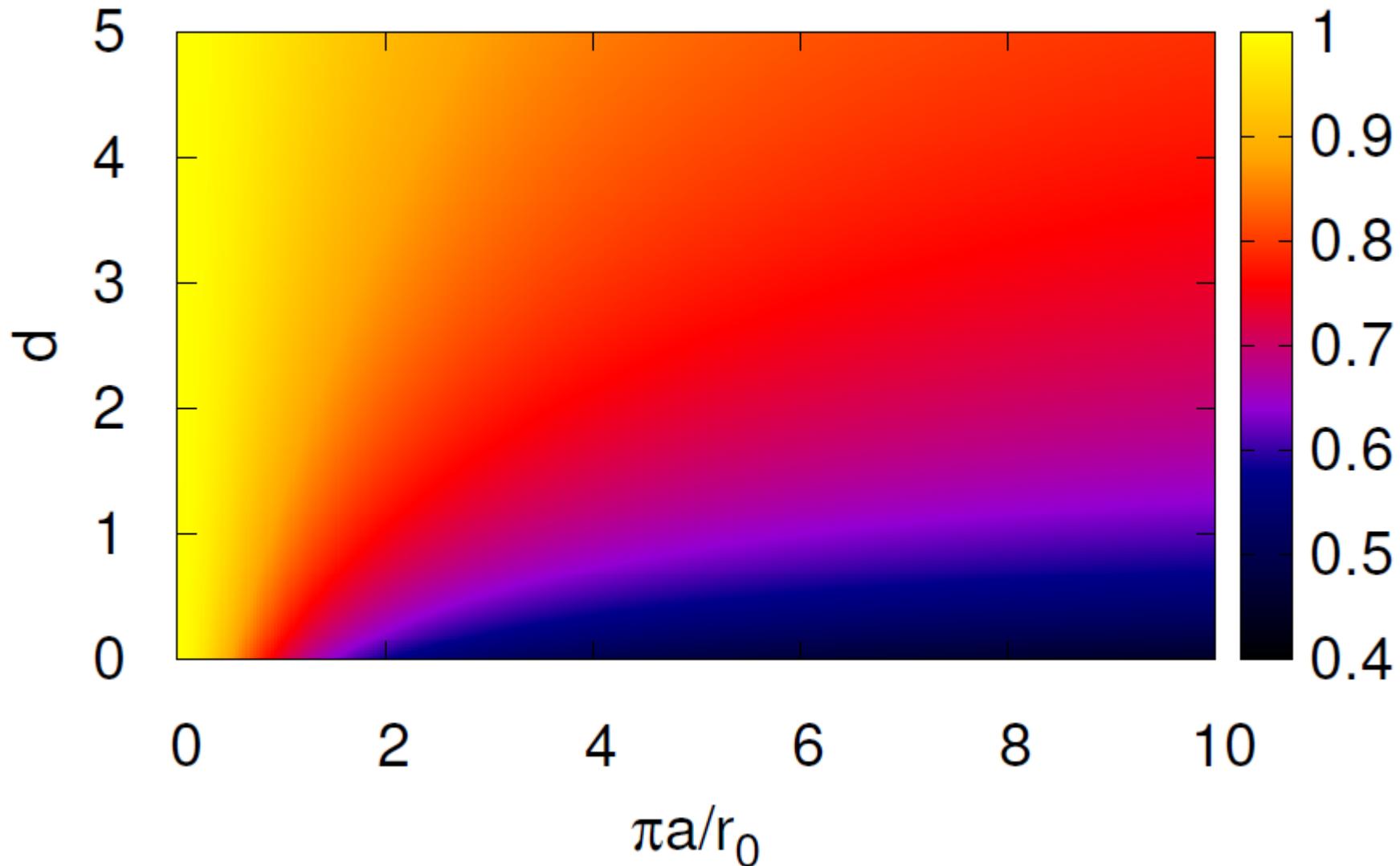
(exciton-exciton interaction)





Wannier model, n=1 state

## Renormalization of QP part



## → Why are we here?

1. Good descriptor: density  $n(r)$  → DFT

So, first we have to calculate the density

**Exact**

2. Auxiliary system for density → KS-DFT

So, first we have to calculate the xc potential

3. Model system → LDA

$$v_{\text{xc}}([n], r) \approx v_{\text{xc}}^{\text{HEG}}(n_r^h)$$

$$v_{\text{xc}}([n], r) = v_{\text{xc}}^{\text{HEG}}(n_r^h)$$

$$n_r^h = n(r)$$

$$n_r^h \approx n(r)$$

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## → Auxiliary system theory

1. Good descriptor: density  $n(r)$  → DFT

So, first we have to calculate the density

**Exact**

2. Auxiliary system for **quantity Q**

**Exact**

So, first we have to calculate the aux. pot., interaction,...

3. Model system → LDA

$$v_{\text{xc}}([n], r) \approx v_{\text{xc}}^{\text{HEG}}(n_r^h)$$

$$v_{\text{xc}}([n], r) = v_{\text{xc}}^{\text{HEG}}(n_r^h)$$

$$n_r^h = n(r)$$

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## → Auxiliary system theory

1. Good descriptor: density  $n(r)$  → DFT

So, first we have to calculate the density

**Exact**

2. Auxiliary system for **quantity Q**

**Exact**

So, first we have to calculate the **aux. pot., interaction,...**

3. Model system → LDA

$$v_{\text{xc}}([n], r) \approx v_{\text{xc}}^H(\mathbf{Exact}) \quad v_{\text{xc}}([n], r) = v_{\text{xc}}^{HEG}(n_r^h)$$

$$n_r^h = \mathbf{Approximation} \quad n_r^h \approx n(r)$$

## → Auxiliary system + Connector theory

1. Good descriptor: density  $n(r)$  → DFT

So, first we have to calculate the density

**Exact**

2. Auxiliary system for **quantity Q**

**Exact**

So, first we have to calculate the aux. pot., interaction,...

3. Model system

→ **Connector Approximation**

**(Exact)**

$$V_{\text{aux}}^{\text{real}}([n], x) = V_{\text{aux}}^{\text{HEG}}(n^h, \tilde{x})$$

$n_r^h =$  **Approximation**

$n^h = ???$