Combining many-body perturbation theory and TD DFT: getting the best of both worlds

TDDFT and Many-Boby Perturbation Theory: comparisons and combinations

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This was 20 years ago!

Today, one of the big challenges of theoretical condensed matter physics is to find ways for describing accurately and efficiently the response of electrons to an external perturbation. In fact, the knowledge of response functions allows one to directly derive spectra (such as absorption or electron energy loss); moreover, response functions enter the description of correlation effects, for example through the screened Coulomb interaction W in Hedin's GW approximation to the electron self-energy. Two main developments for the *ab initio* calculation of response functions of both finite and infinite systems are, on one side, the solution of the Bethe-Salpeter equation (BSE), and, on the other hand, Time-Dependent Density Functional Theory (TDDFT). Both approaches are promising, but suffer from different shortcomings: the solution of the Bethe-Salpeter equation is numerically very demanding, whereas for TDDFT, despite recent progress a generally reliable but at the same time very efficient description of exchange-correlation effects has still to be developed.

We will review the two approaches focussing on their comparison. The meaning and importance of different contributions to the induced potentials will be analyzed for various systems, ranging from atoms to bulk semiconductors and insulators, from graphite to nanotubes. We will then show various ways to combine TDDFT and the BSE approach, that are all leading to a similar class of exchange-correlation kernels. These kernels yield excellent results for absorption and energy loss spectra; moreover, they can be used to determine vertex corrections beyond the GW approximation. We will discuss the links between these methods as well as the relation with other work (in particular, with a perturbation theory picture, and with the exact-exchange approach), show results and give perspectives.

Combining many-body perturbation theory and TD DFT: getting the best of both worlds

Marc Aichner, Ayoub Aouina, Abdallah El Sahili, Matteo Gatti, Jaakko Koskelo,
Elena Martini, Martin Panholzer, Claudia Roedl, Francesco Sottile, Marilena Tzavala,
Lucia Reining

This kept us busy for 20 years!

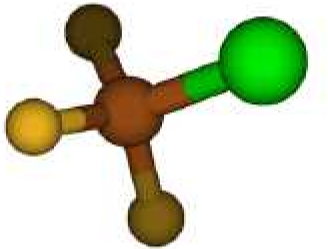
ETSF

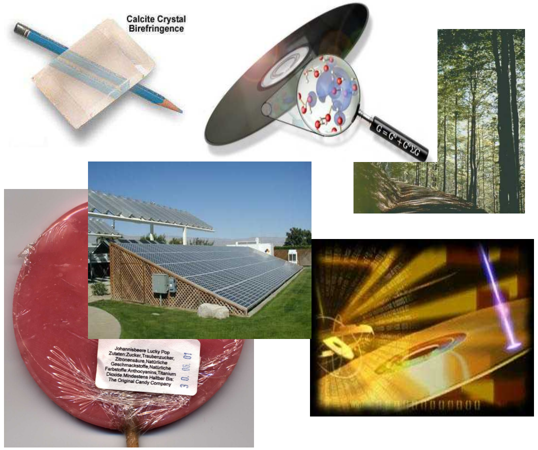
ÉCOLE POLYTECHNIQUE

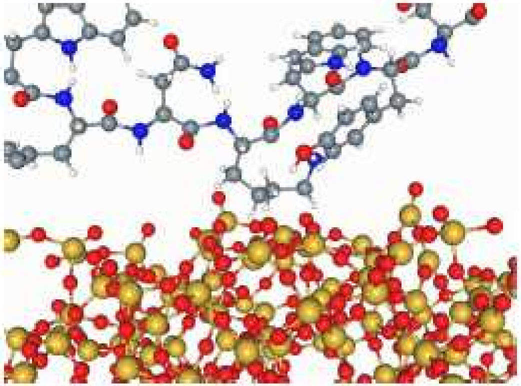
IP PARIS

Combining many-body perturbation theory and TD DFT: getting the best of both worlds

$\Psi(x_1, x_2, ..., x_N; t)$	$G(x_1, x_1', t, t')$	$n(\mathbf{r}; t)$
$O = O[\Psi]$	$O = \tilde{O}[\underbrace{Q}_{G}]$	$O = \tilde{O}[\underbrace{Q}_{n}]$
CI, QMC	Green's Functions	Density Functionals







Combining many-body perturbation theory and TD DFT: getting the best of both worlds

MBPT = GFFT   DFT

$$\text{TD-GFFT} \longrightarrow \chi \longleftarrow \text{TD-DFT}$$

Combining many-body perturbation theory and TD DFT: getting the best of both worlds

A simplified view:

MBPT = GFFT — DFT

TD-GFFT $\longrightarrow \chi \longleftarrow$ TD-DFT

“easy to approximate” — ”easy to calculate”

Combining many-body perturbation theory and TD DFT: getting the best of both worlds

A simplified view:

MBPT = GFFT DFT

TD-GFFT $\longrightarrow \chi \longleftarrow$ TD-DFT

"easy to approximate" "easy to calculate"

(which is of course only true when quick&dirty)

$\Rightarrow$ **Merge and keep the best of both worlds**

Combining many-body perturbation theory and TDDFT: getting the best of both worlds

→ Historical examples in modern perspective:

* TDDFT from the Bethe-Salpeter equation of MBPT

* vertex corrections beyond GW from TDDFT

→ Our today's research:

* fxc approx. vertex corrections: exotic excitations in the HEG

* How wrong are fxc approx. vertex corrections *in principle?*

→ A central quantity: $\Sigma[n]$

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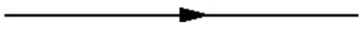
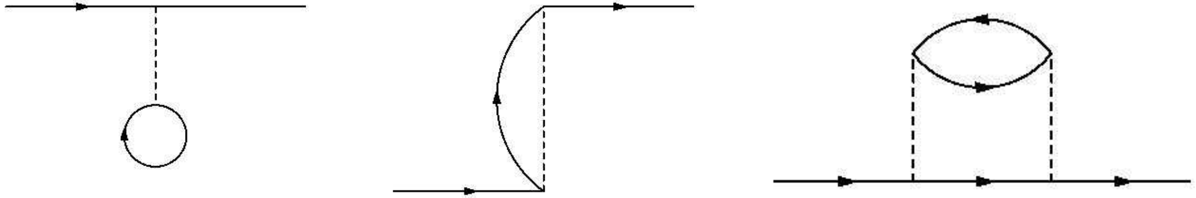
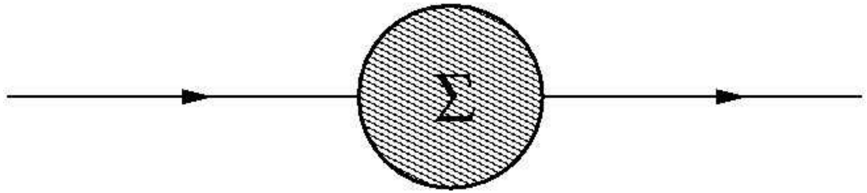
Typical GFFT approximation strategy

$$G(x_1, x_1', t, t') = -i\langle N|T[\hat{\Psi}(x_1, t)\hat{\Psi}^\dagger(x_1', t')]|N\rangle$$





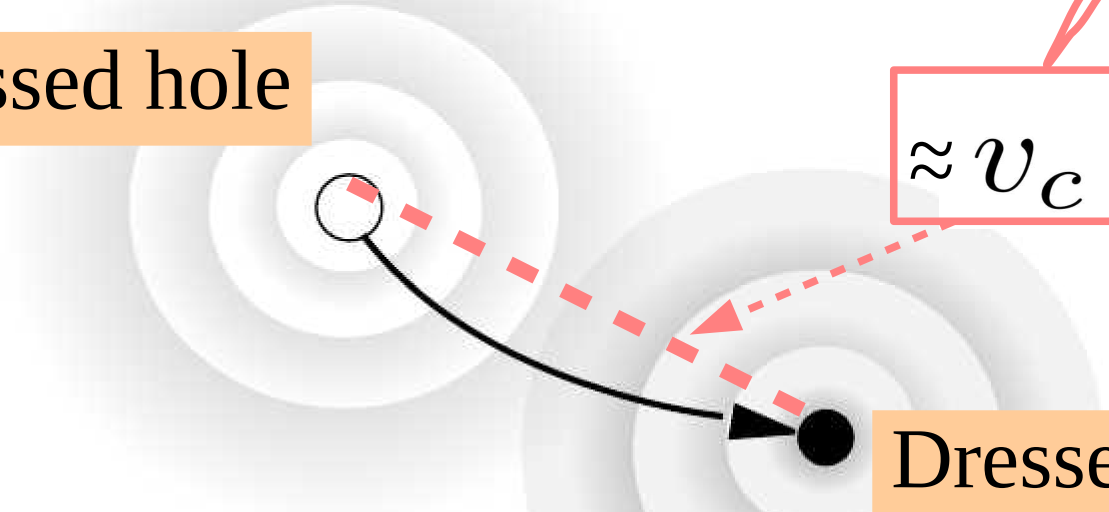


Dyson equation: $G = G_0 + G_0 \Sigma G$

Bethe-Salpeter Equation

$$L = L_0 + L_0 \underbrace{\frac{\delta(v_H + \Sigma_{\mathrm{xc}})}{\delta G}}_{\boxed{\approx v_c \; - \; W}} L$$

$$L_0 = GG$$



Hanke & Sham, Phys. Rev. Lett. 43, 387 (1979)
Strinati, Nuovo Cimento 11, 1 (1988)
Onida, et al., Phys. Rev. Lett. 75, 818 (1995)
Albrecht, Onida, Reining Phys. Rev. B 55, 10278 (1997); Albrecht et al. PRL 80, 4510 (1998)
Benedict, Shirley, Bohn, PRL 80, 4514 (1998)
Rohlfing & Louie, PRL 80, 3320 (1998); PRL 81, 2312 (1998)

Why do we use the BSE?

$$\chi = \frac{\delta n}{\delta v_{\mathrm{ext}}}$$

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$$\chi = \frac{\delta n}{\delta v_{\mathrm{ext}}} = \frac{\delta n}{\delta v_{\mathrm{tot}}} \frac{(\delta v_{\mathrm{ext}} + \delta v_{\mathrm{H}} + \delta v_{\mathrm{xc}})}{\delta v_{\mathrm{ext}}}$$

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LR-TDDFT

$$\chi = \chi^0 + \chi_0 \left(\frac{\delta v_{\rm H} + \delta v_{\rm xc}}{\delta n} \right) \frac{\delta n}{\delta v_{\rm ext}}$$

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Approximations not reliable in extended systems $\rightarrow$ switch to GF

Now the total potential contains $\Sigma(\mathbf{r}, \mathbf{r}', \omega; [G])$, e.g. $v_{\mathrm{H}} + iGW$

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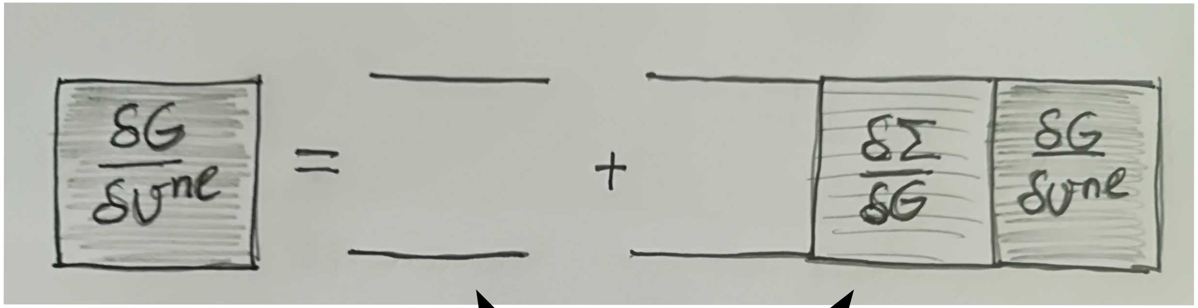
$$L = \frac{\delta G}{\delta v_{\mathrm{ext}}} = \frac{\delta G}{\delta v_{\mathrm{tot}}} \frac{(\delta v_{\mathrm{ext}} + \delta v_{\mathrm{H}} + \delta \Sigma_{\mathrm{xc}})}{\delta G} \frac{\delta G}{\delta v_{\mathrm{ext}}}$$

$$L_0 \equiv GG$$

$$L = L_0 + L_0 \left(-iv_c + \frac{\delta \Sigma_{\mathrm{xc}}}{\delta G} \right) L$$

Standard approximation to BSE:



GW

W is input
Instantaneous approx in e-h interaction
QP approx for G

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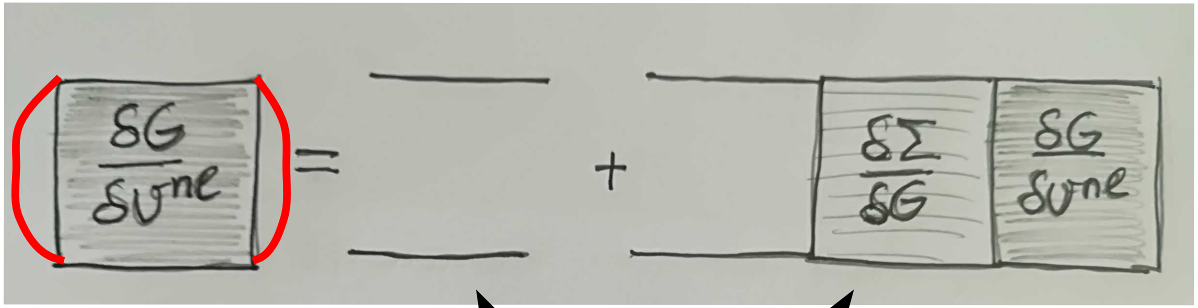


GW

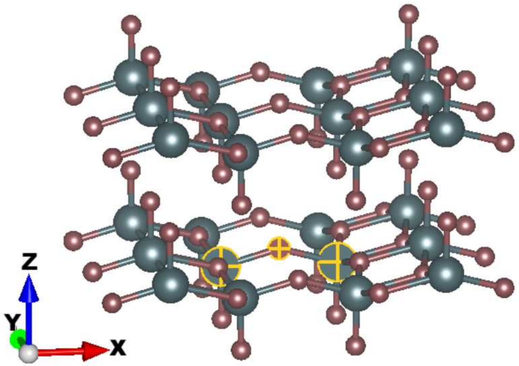
W is input
Instantaneous approx in e-h interaction
QP approx for G

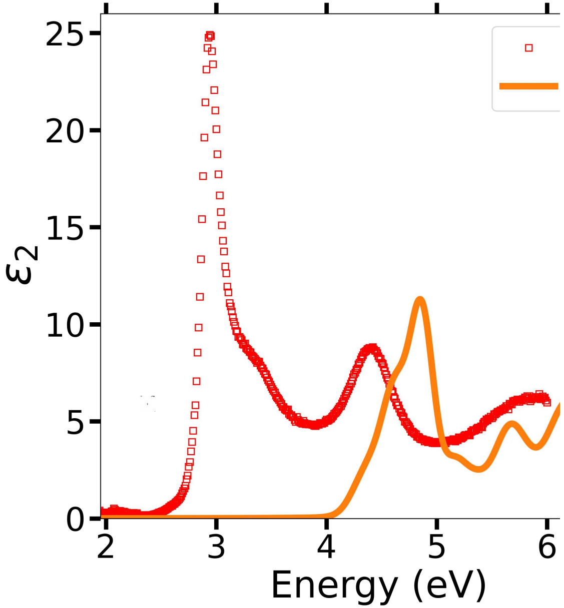
Solve BSE, then get χ from $n(\mathbf{r}) = -iG(\mathbf{r}, \mathbf{r}, t, t^{+})$

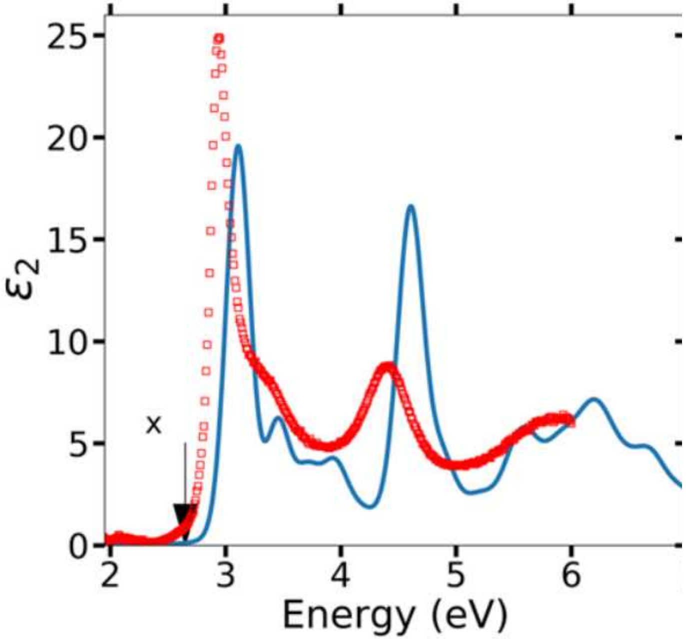
Optical absorption

Chaire Énergies Durables
École polytechnique - EDF

V_2O_5: a layered bulk material







GW-RPA

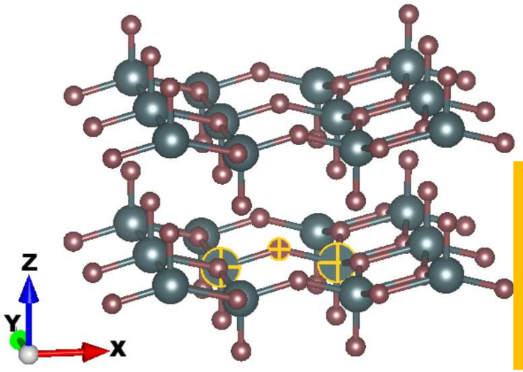
Exp

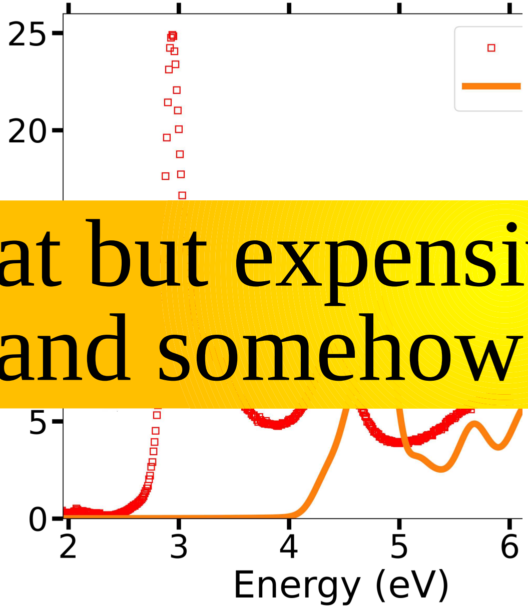
BSE

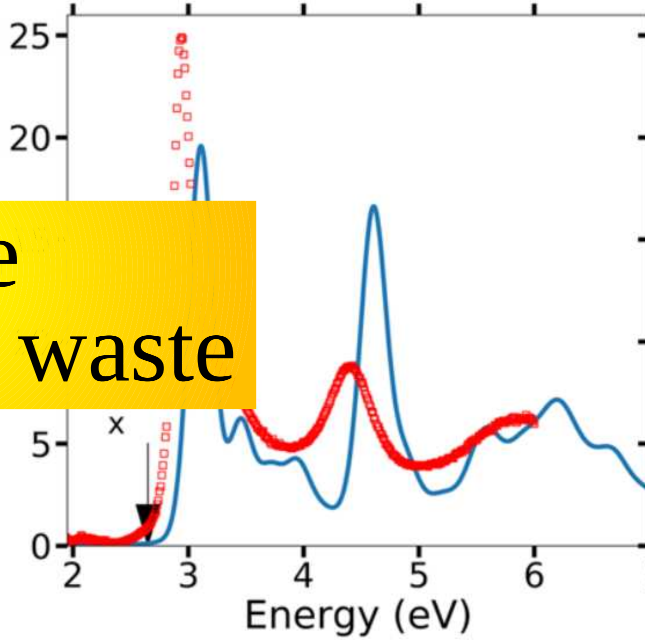
Vitaly Gorelov
Reining, Feneberg, Goldhahn, Schleife, Lambrecht, Gatti
npj comp mat 8,94 (2022)

Optical absorption

V_2O_5: a layered bulk material







Great but expensive
…..and somehow a waste

GW-RPA

Exp

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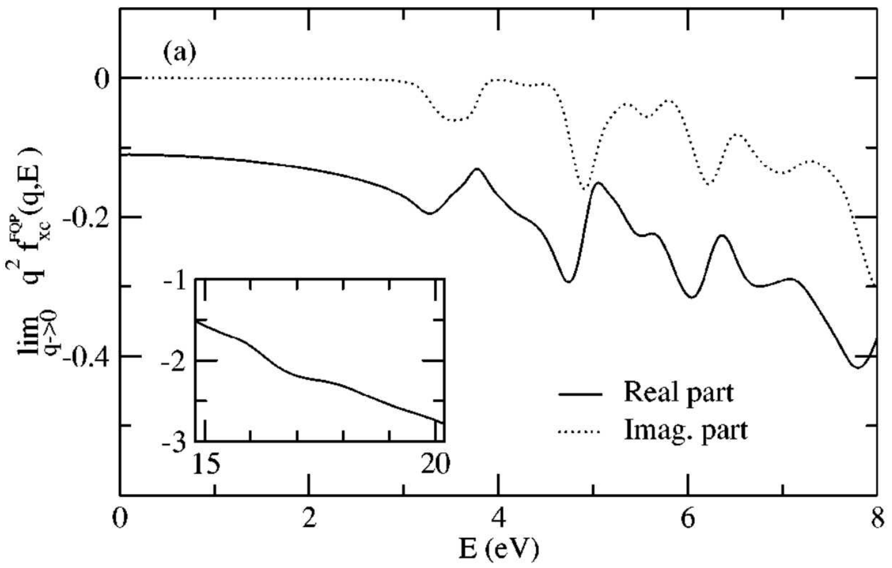
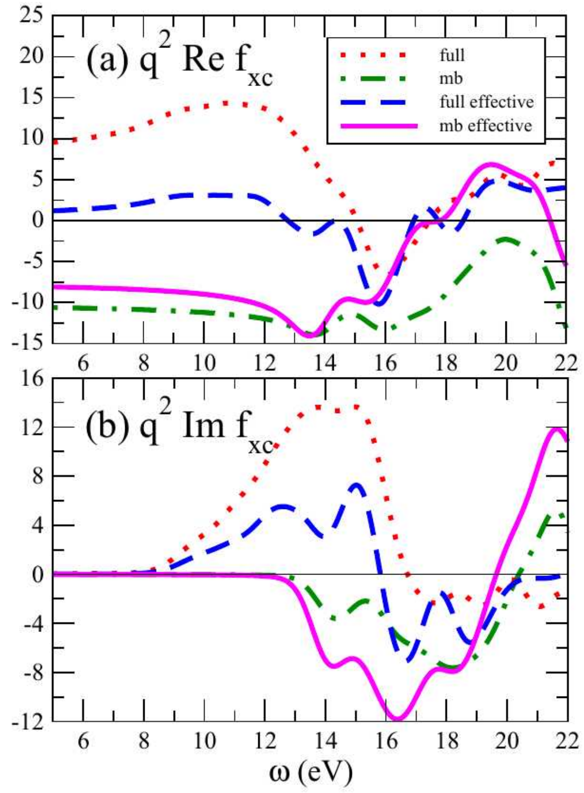
From the BSE to a kernel for TDDFT: reverse engineering



Del Sole et al., PRB 67, 045207 (2003): Silicon, (diamond)

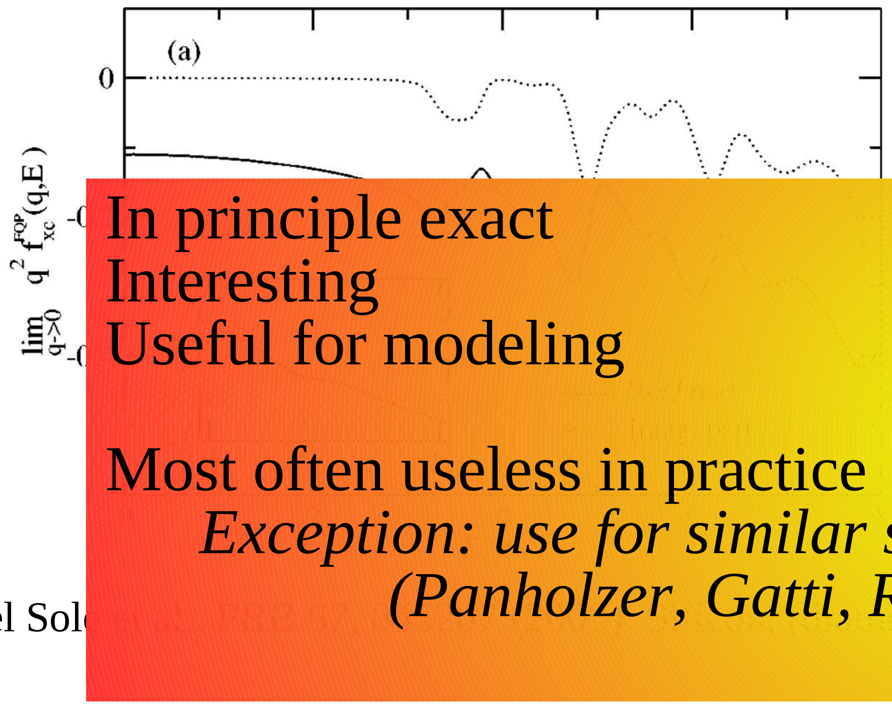


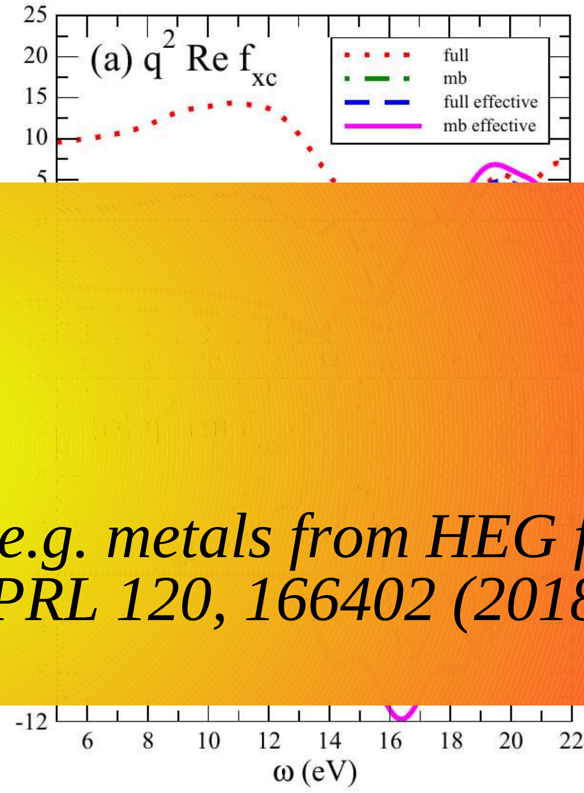
Reshetnyak, et al., PR Research 1, 032010(R) (2019)

LiF

$$\chi = \chi^{\mathrm{RPA}} + \chi^{\mathrm{RPA}} f_{\mathrm{xc}} \chi$$

From the BSE to a kernel for TDDFT: reverse engineering





Reshetnyak, et al., PR Research 1, 032010(R) (2019):

In principle exact
Interesting
Useful for modeling

Most often useless in practice

Exception: use for similar systems, e.g. metals from HEG fxc(ω)
(Panholzer, Gatti, Reining, PRL 120, 166402 (2018))

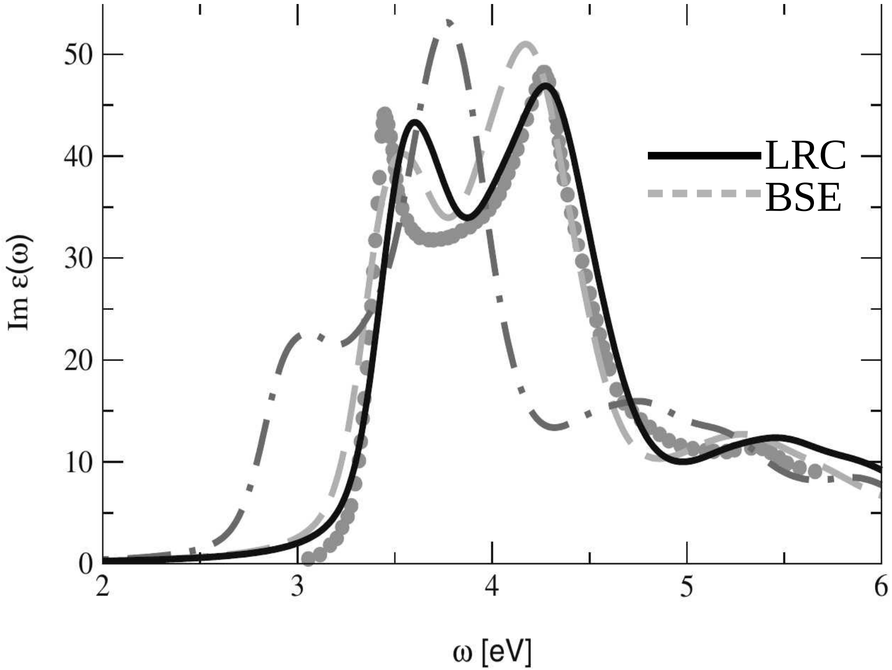
Del Sol

$$\chi = \chi^{\mathrm{RPA}} + \chi^{\mathrm{RPA}} f_{\mathrm{xc}} \chi$$

From the BSE to a kernel for TDDFT: reverse engineering by (dirty) maths

→ Approx:

$$f_{\rm xc}(\mathbf{q}, \mathbf{G}, \mathbf{G}') = -\delta_{\mathbf{G},\mathbf{G}'}\alpha/|\mathbf{q} + \mathbf{G}|^2$$



Reining , et al., PRL 88, 066404 (2002): silicon

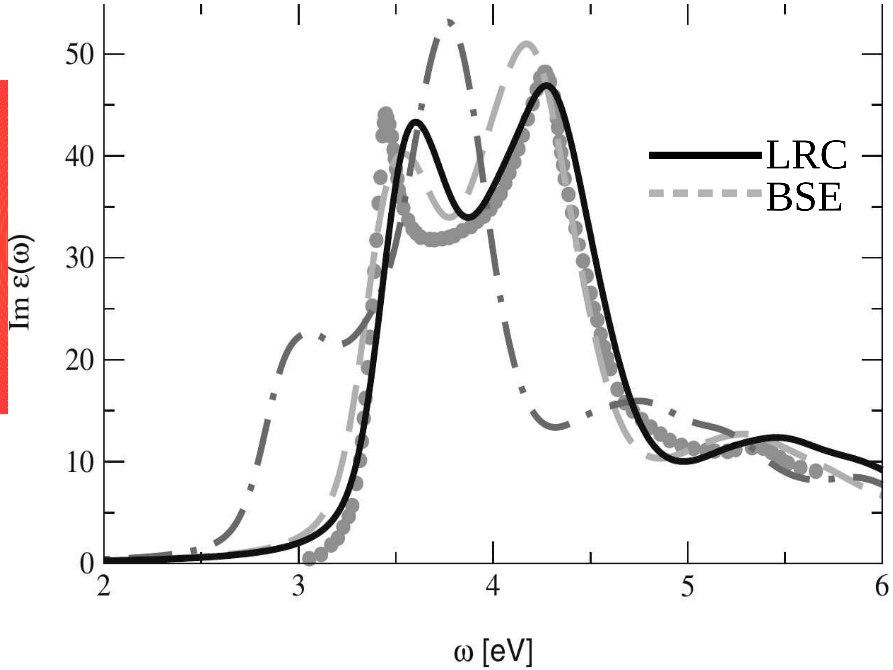
From the BSE to a kernel for TDDFT: reverse engineering by (dirty) maths

→ Approx:

$$f_{xc}(\mathbf{q},\mathbf{G},\mathbf{G}') = -\delta_{\mathbf{G},\mathbf{G}'}\alpha/|\mathbf{q}+\mathbf{G}|^2$$

Exact in some limit
Interesting
Useful for modeling

Not good for bound excitons



Reining , et al., PRL 88, 066404 (2002): silicon

$$\chi = \frac{\delta n}{\delta v_{\text{ext}}} = \frac{\delta n}{\delta v_{\text{tot}}} \frac{(\delta v_{\text{ext}} + \delta v_{\text{H}} + \delta \Sigma_{\text{xc}})}{\delta G} \frac{\delta G}{\delta v_{\text{ext}}}$$

$$\begin{aligned}
\Sigma_{\text{xc}}^{\text{GW}}(\mathbf{r}, \mathbf{r}', t, t') &= iG(\mathbf{r}, \mathbf{r}', t, t') W(\mathbf{r}', \mathbf{r}, t', t^+) \\
&\approx iG(\mathbf{r}, \mathbf{r}', t, t') W(\mathbf{r}', \mathbf{r}, \omega = 0) \delta(t' - t^+) \\
&= -\rho(\mathbf{r}, \mathbf{r}') W(\mathbf{r}', \mathbf{r}, \omega = 0) \delta(t' - t^+)
\end{aligned}$$

"our" BSE $$\frac{\delta \rho}{\delta v_{\text{ext}}} = \frac{\delta \rho}{\delta v_{\text{tot}}} \left(1 + \frac{(\delta v_{\text{H}} + \delta \Sigma_{\text{xc}})}{\delta \rho} \frac{\delta \rho}{\delta v_{\text{ext}}}\right)$$

Onida, Reining, Rubio
RMP 74, 601 (2002)

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$$\Sigma_{\rm xc}^{\rm GW}(\mathbf{r}, \mathbf{r}', t, t') = iG(\mathbf{r}, \mathbf{r}', t, t')W(\mathbf{r}', \mathbf{r}, t', t^+)$$

$$\approx iG(\mathbf{r}, \mathbf{r}', t, t')W(\mathbf{r}', \mathbf{r}, \omega = 0)\delta(t' - t^+)$$

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$$\chi = \chi_0 + \chi_0^3\frac{(\delta v_{\mathrm{H}} + \delta\Sigma_{\mathrm{xc}})}{\delta\rho}\frac{\delta\rho}{\delta n}\chi$$

In principle we are not forced to terminate with the 1RDM

$$\frac{\delta\rho}{\delta v_{\mathrm{ext}}} = \frac{\delta\rho}{\delta v_{\mathrm{tot}}}(1 + \frac{(\delta v_{\mathrm{H}} + \delta\Sigma_{\mathrm{xc}})}{\delta\rho}\frac{\delta\rho}{\delta v_{\mathrm{ext}}})$$

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This is TDDFT-like ("many-body effective")

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But we had to approximate this derivative…..

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But we had to approximate this derivative….. → Nanoquanta kernel

Sottile, Olevano, Reining, PRL 91, 056402 (2003)

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$$\chi = \chi_0 + \chi_0^3 \frac{(\delta v_{\text{H}} + \delta\Sigma_{\text{xc}})}{\delta\rho}\frac{\delta\rho}{\delta n}\chi$$

Interesting

Expensive
Delicate

This is TDDFT-like (“many-body effective”)

But we had to approximate this derivative….. → Nanoquanta kernel

Sottile, Olevano, Reining, PRL 91, 056402 (2003)

$$\frac{\delta\rho}{\delta v_{\mathrm{ext}}} = \frac{\delta\rho}{\delta v_{\mathrm{tot}}}(1 + \frac{(\delta v_{\mathrm{H}} + \delta\Sigma_{\mathrm{xc}})}{\delta\rho}\frac{\delta\rho}{\delta v_{\mathrm{ext}}})$$

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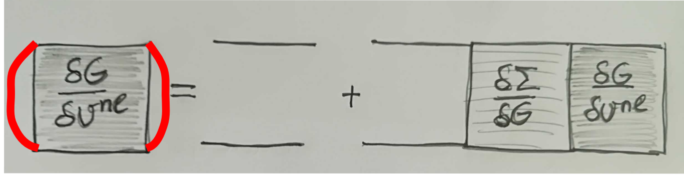
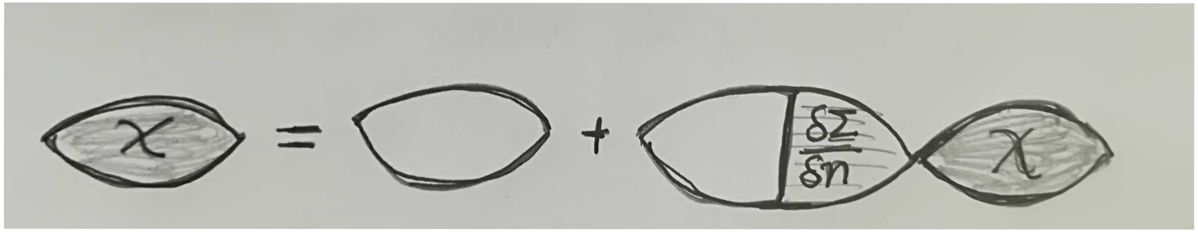
Bruneval, Sottile, Olevano, Del Sole, Reining
Phys. Rev. Lett. 94, 186402 (2005)

We could also avoid $\rho[n] \longrightarrow \Sigma = \Sigma[n]$





$$\chi = \chi_0 + \chi_0^3 \frac{(\delta v_{\mathrm{H}} + \delta\Sigma_{\mathrm{xc}})}{\cancel{\delta\rho}} \frac{\cancel{\delta\rho}}{\delta n} \chi$$

Bruneval, Sottile, Olevano, Del Sole, Reining
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We could also avoid $\rho[n] \longrightarrow \Sigma = \Sigma[n]$ To be approximated!!!

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→ Historical examples in modern perspective:

* fxc from the Bethe-Salpeter equation of MBPT

* vertex corrections beyond GW from TDDFT

→ Our today's research:

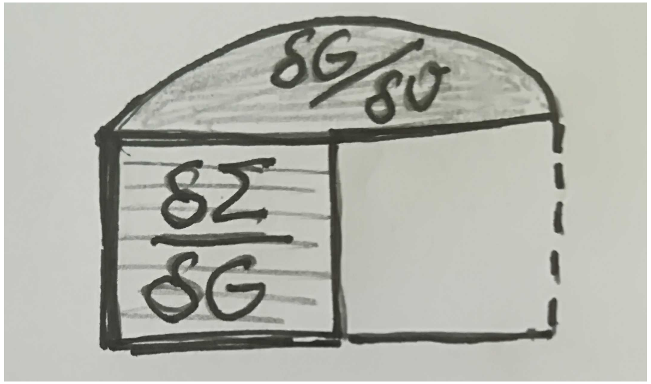
* fxc approx. vertex corrections: exotic excitations in the HEG

* How wrong are fxc approx. vertex corrections *in principle?*

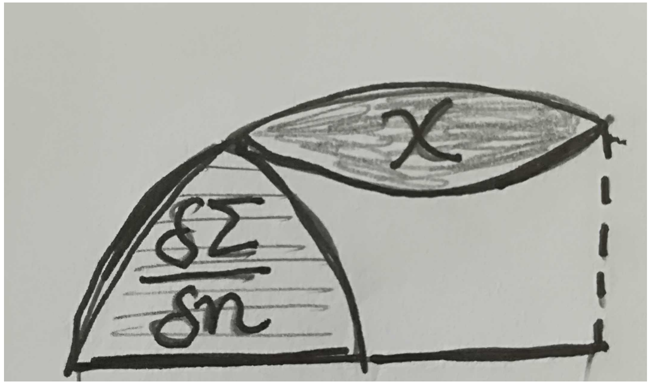
→ A central quantity: Σ[n]

From TDDFT to vertex corrections beyond GW

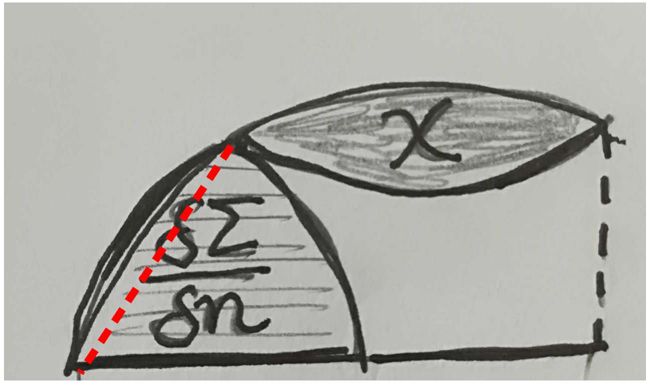
Correlation self-energy:



Martin, Reining, Ceperley
Interacting Electrons
(Cambridge 2016)



Bruneval, et al,
PRL 94, 186402 (2005)

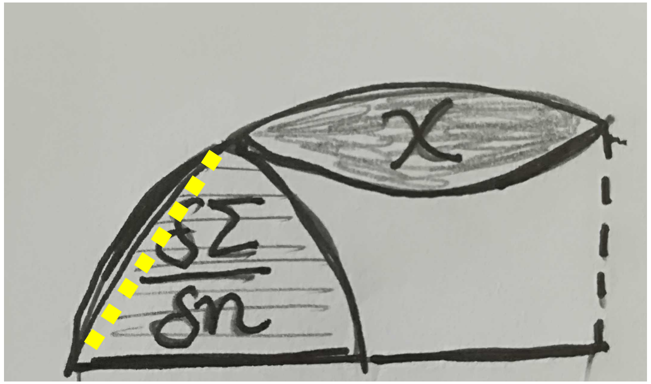


GW
Hedin 1965

$$\frac{\delta\Sigma}{\delta G}\frac{\delta G}{\delta v} = \frac{\delta\Sigma}{\delta n}\frac{\delta n}{\delta v} = \left(v_c + \cancel{\frac{\delta\Sigma_{\mathrm{xc}}}{\delta n}}\right)\chi$$

From TDDFT to vertex corrections beyond GW

"G$\tilde{W}$"



$= v_c + f_{\rm xc}$

Beyond GW, approximate vertex from TDDFT: $i\dfrac{\delta\Sigma_{\rm xc}}{\delta G} \rightarrow \dfrac{\delta v_{\rm xc}}{\delta n} = f_{\rm xc}$

Overhauser, PRB 3, 1888 (1971); Streitenberger, Phys. Stat. Sol. 125, 681 (1984); Phys. Lett. 106A, 57 (1984);
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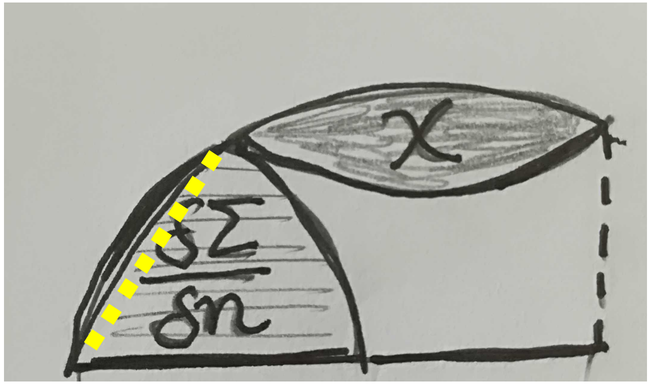
Shishkin, Marsman, and Kresse, PRL 99, 246403 (2007).

From TDDFT to vertex corrections beyond GW

"G$\widetilde{\text{W}}$"

	GW RPA	GW K_{xc}	$GW\Gamma$
Direct gap at Γ	0.64	0.56	0.65
Direct gap at X	0.78	0.57	0.73
Direct gap at L	0.68	0.58	0.72
Valence bandwidth	-0.56	-1.01	-0.48
Minimum gap	0.63	0.59	0.66
Valence band maximum	-0.36	-0.44	0.01
Conduction band minimum	0.27	0.14	0.67

$= v_c + f_{xc}$



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Conduction band minimum	0.27	0.1[illegible]	[illegible]

$= v_c + f_{xc}$

Interesting

NOT in principle exact
Systematic?
Usefulness in practice?

Beyond GW, approximate vertex from TDDFT: $i\dfrac{\delta \Sigma_{xc}}{\delta G} \to \dfrac{\delta v_{xc}}{\delta n} = f_{xc}$

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Combining many-body perturbation theory and TDDFT: getting the best of both worlds

→ Historical examples in modern perspective:

* fxc from the Bethe-Salpeter equation of MBPT

* vertex corrections beyond GW from TDDFT

Jaakko Koskelo

→ Our today's research:

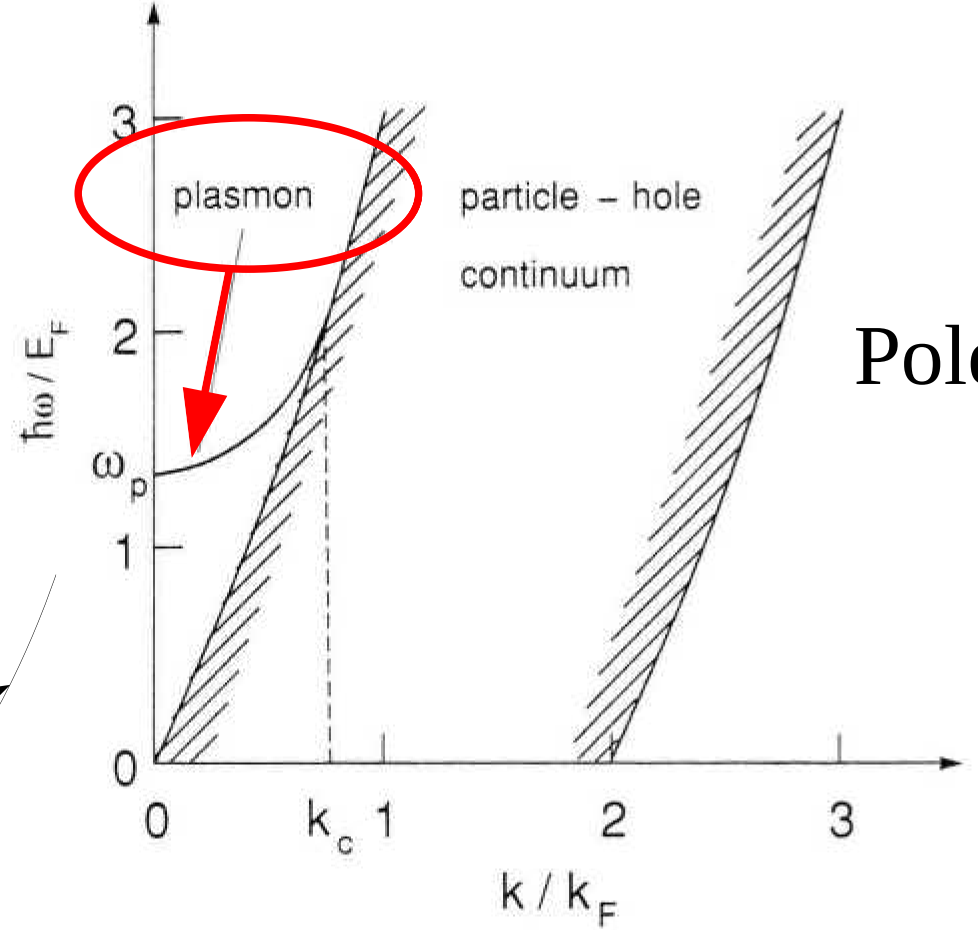
* fxc approx. vertex corrections: exotic excitations in the HEG

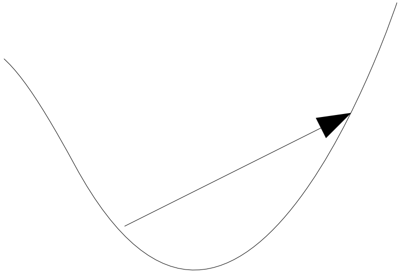
* How wrong are fxc approx. vertex corrections *in principle?*

→ A central quantity: $\Sigma[n]$

Excitations in the homogeneous electron gas

collective



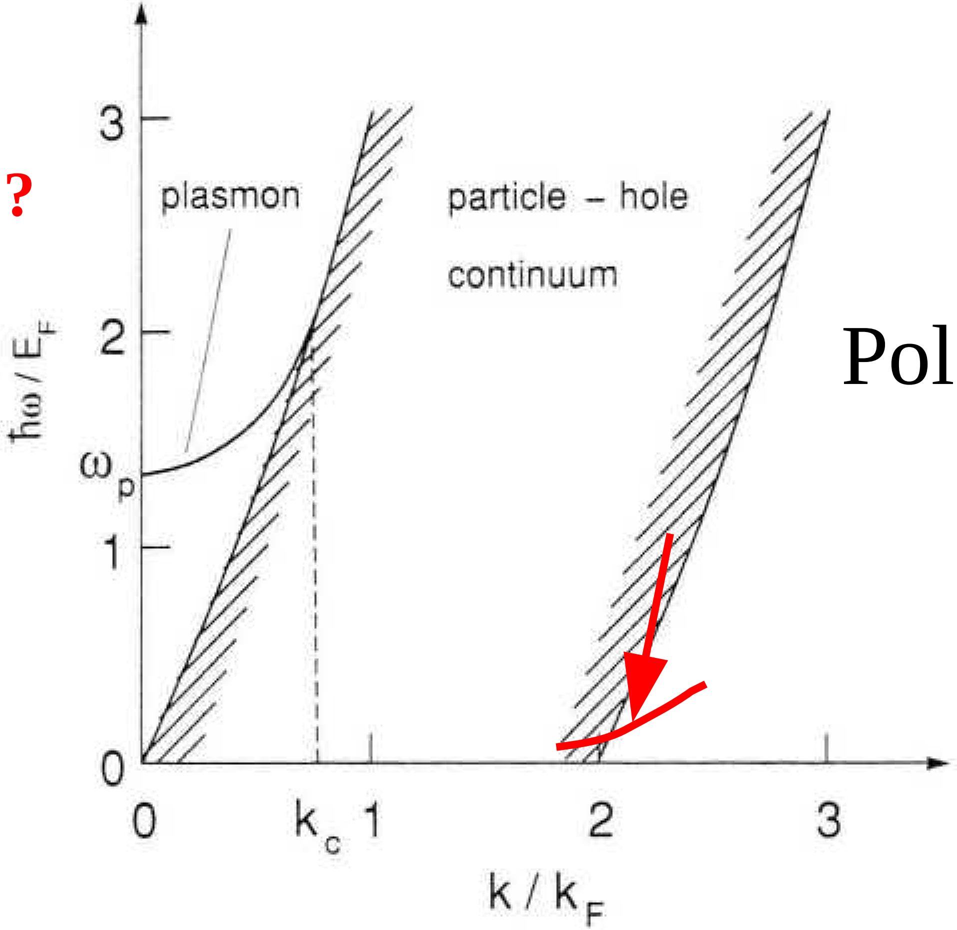


Poles in χ (from L)

from K. Sturm, “Dynamic Structure Factor: an Introduction”, Zeitschrift für Naturforschung A (1993)

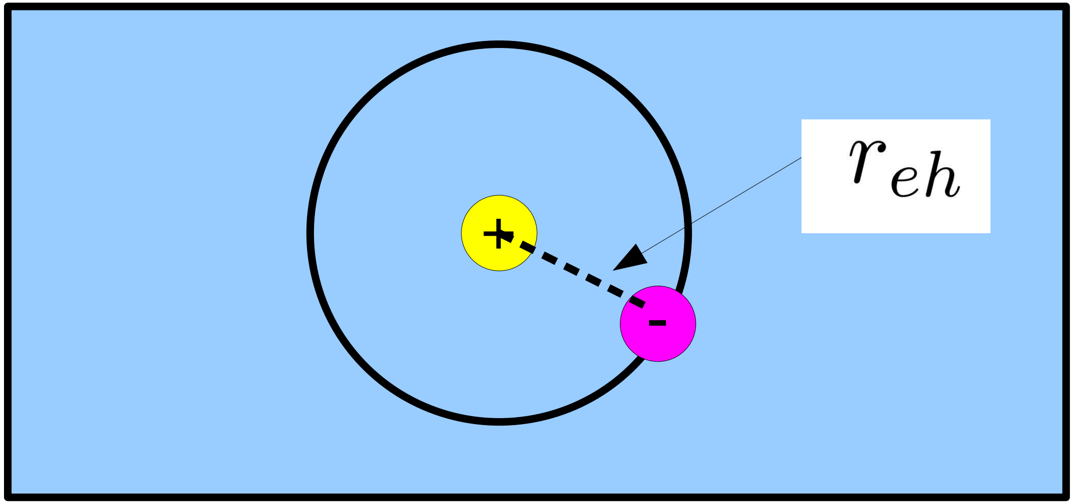
Excitations in the homogeneous electron gas

Collective???



Poles in χ (from L)

Textbook knowledge



Wannier exciton:

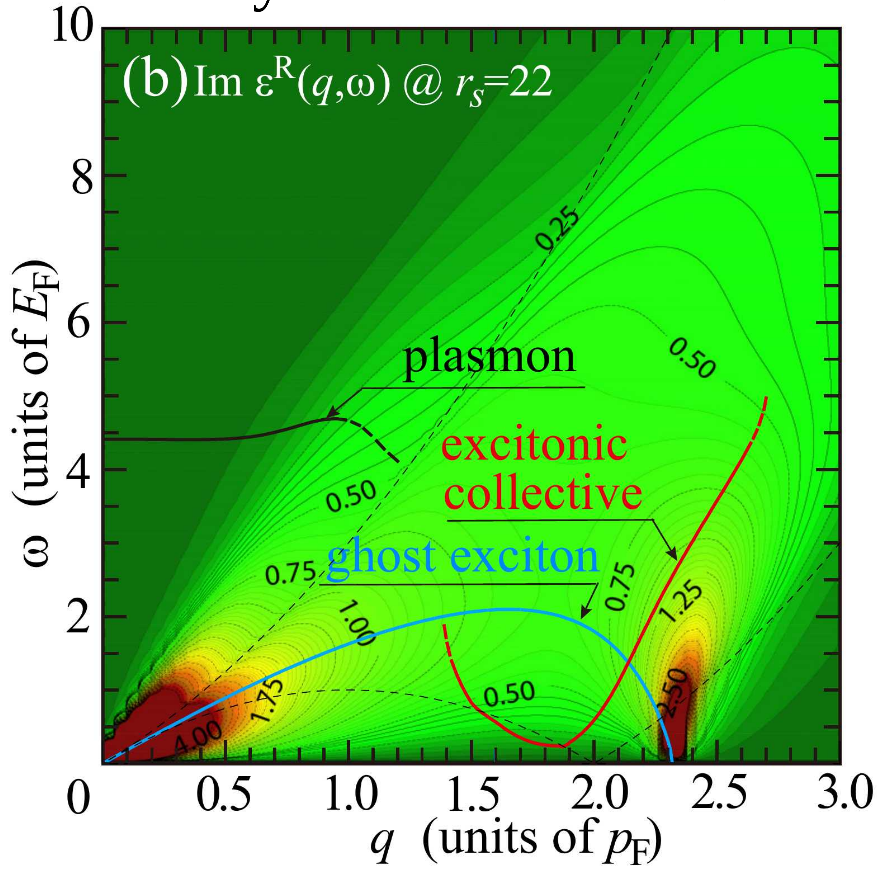
$$E_B \propto \frac{\mu}{\epsilon^2 n^2}$$

$$\frac{1}{\mu} = \frac{1}{m_e} + \frac{1}{m_h}$$

$$r_{eh} = \frac{\epsilon}{\mu} n^2 a_0$$

Intuitively: excitons screened out in the HEG

But at low density…... Y. Takada, PRB 94, 245106 (2016)



See also: Takayanagi&Lipparini, PRB 56, 4872 (1997)

What is a ghost mode?

What is a ghost mode?

$$v_{\text{tot}}(\omega) = \epsilon^{-1}(\omega) v_{\text{ext}}(\omega)$$

$$\epsilon^{-1}(\omega) = 1 + v_c \chi(\omega)$$

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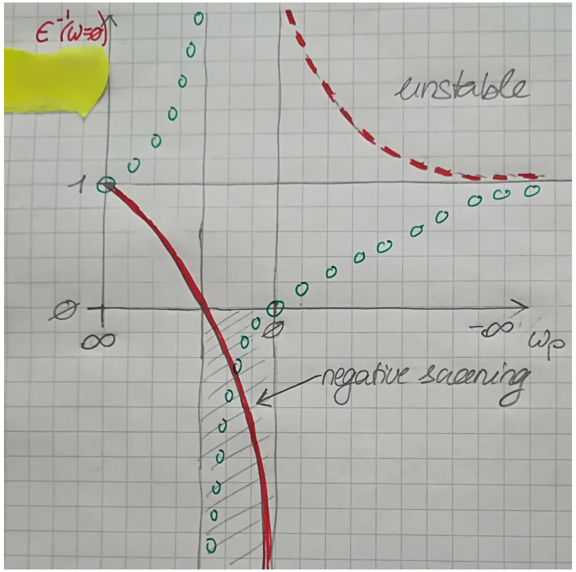
$$\boxed{\begin{aligned} v_{\text{tot}}(\omega) &= \epsilon^{-1}(\omega) v_{\text{ext}}(\omega) \\ \epsilon^{-1}(\omega) &= 1 + v_c \chi(\omega) \end{aligned}}$$

$$\chi(\omega) = a \frac{2\omega_p}{\omega^2 - \omega_p^2} \qquad \epsilon^{-1}(\omega) = 1 + v_c\, a \frac{2\omega_p}{\omega^2 - \omega_p^2}$$

$$\epsilon^{-1}(\omega = 0) = 1 - \frac{2v_c\, a}{\omega_p}$$

< 0 for $\omega_p < 2av_c$



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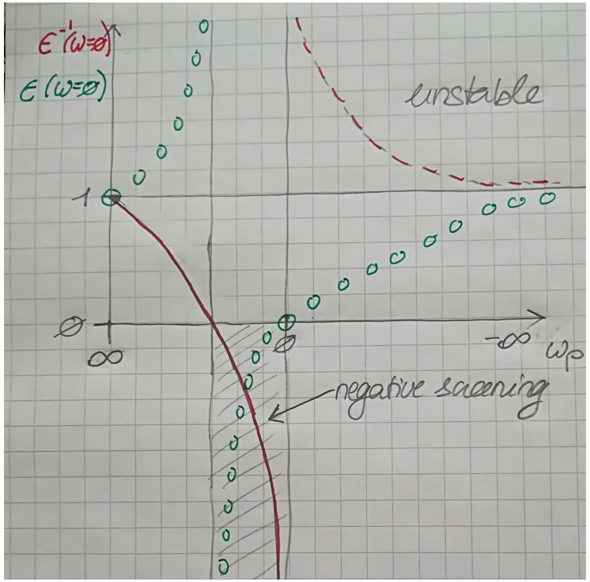
$$\epsilon^{-1}(\omega = 0) = 1 - \frac{2 v_c\, a}{\omega_p}$$

< 0 for $\omega_p < 2 a v_c$

$$\epsilon^{-1}(\omega = 0) < 0 \quad \rightarrow \quad \epsilon(\omega = 0) < 0$$



$$\epsilon(\omega) = \frac{\omega^2 - \omega_p^2}{\omega^2 - \omega_p^2 + 2 a v_c \omega_p}$$

$$\epsilon = 1 - v_c P$$

Pole at $\omega = \pm\sqrt{\omega_p^2 - 2 a v_c \omega_p}$

$$v_{\text{tot}}(\omega) = \epsilon^{-1}(\omega) v_{\text{ext}}(\omega)$$

$$\epsilon^{-1}(\omega) = 1 + v_c \chi(\omega)$$

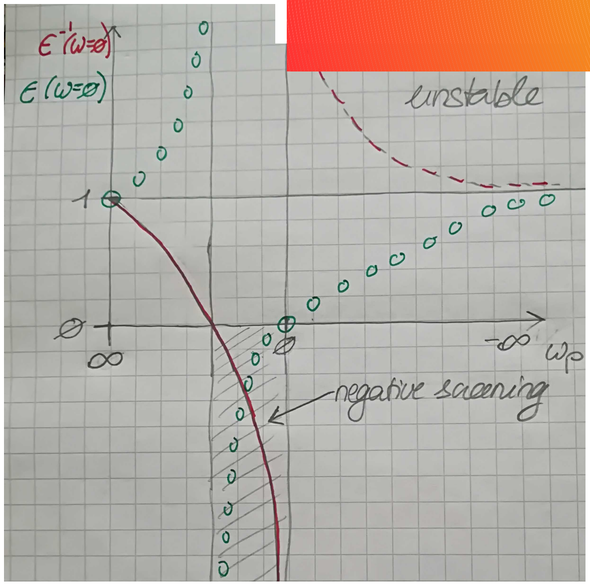
What is a ghost mode?

$\chi(\omega) =$

Low energy excitation → negative screening

Poles of P moving to zero → ghost (imaginary) poles

Precursors for instability !



$$\epsilon^{-1}(\omega = 0) < 0 \quad \rightarrow \quad \epsilon(\omega = 0) < 0$$

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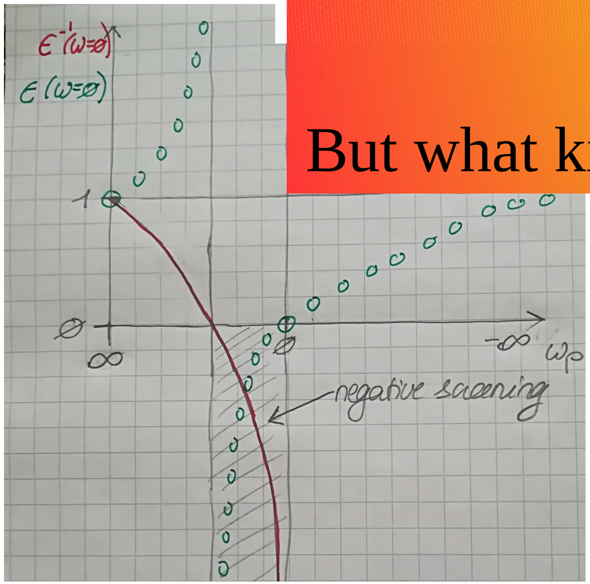
Precursors for instability !

But what kind of excitation is this?

$0) < 0$



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Why should this be important?

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$$\epsilon^{-1}(\omega) = 1 + v_c \chi(\omega)$$

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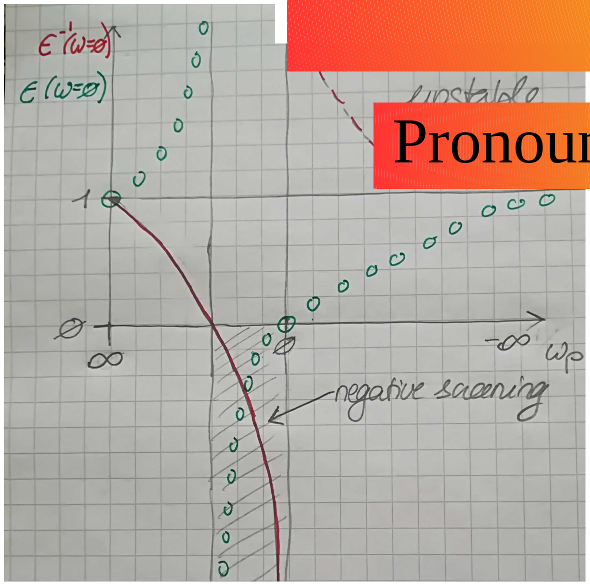

$$\epsilon^{-1}(\omega = 0) < 0 \rightarrow \epsilon(\omega = 0) < 0$$

Pronounced low energy excitation = exciton?

$$\epsilon(\omega) = \frac{\omega^2 - \omega_p^2}{\omega^2 - \omega_p^2 + 2a v_c \omega_p}$$

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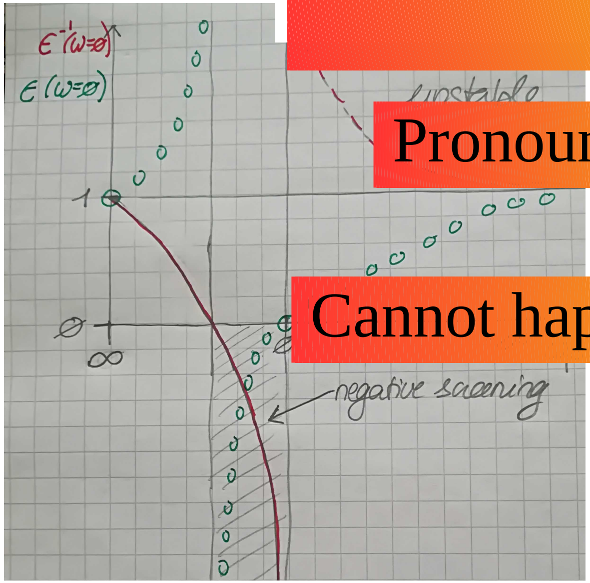


$\epsilon(\omega = 0) < 0$

Pronounced low energy excitation = exciton?

$\omega^2 - \omega_p^2$

Cannot happen with classical electrostatics (the RPA)!!!

$$\epsilon = 1 - v_c P$$

Pole at $\omega = \pm\sqrt{\omega_p^2 - 2 a v_c \omega_p}$

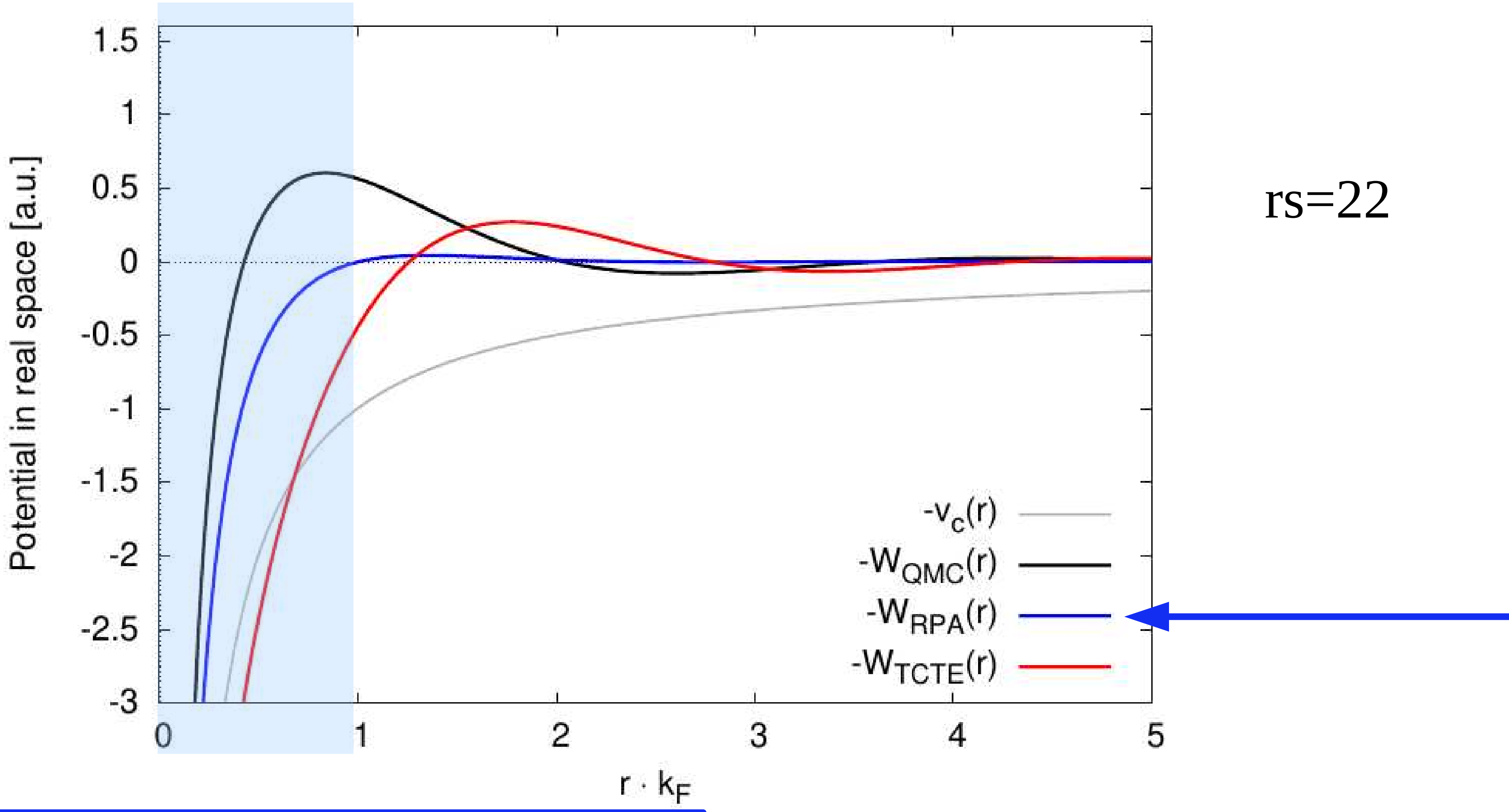
We usually describe excitons in the BSE:

$$\left.\begin{array}{l}\epsilon^{\mathrm{in}}(q) \to \Sigma = iGW^{\mathrm{in}} : \quad \text{e-e repulsion} \\ \epsilon^{\mathrm{in}}(q) \to -W^{\mathrm{in}} \;:\quad \text{e-h attraction}\end{array}\right\} \xrightarrow{\mathrm{BSE}} \epsilon^{\mathrm{out}}(q,\omega)$$

* Static W^{in}

* QP approx

Is the e-h interaction screened away?



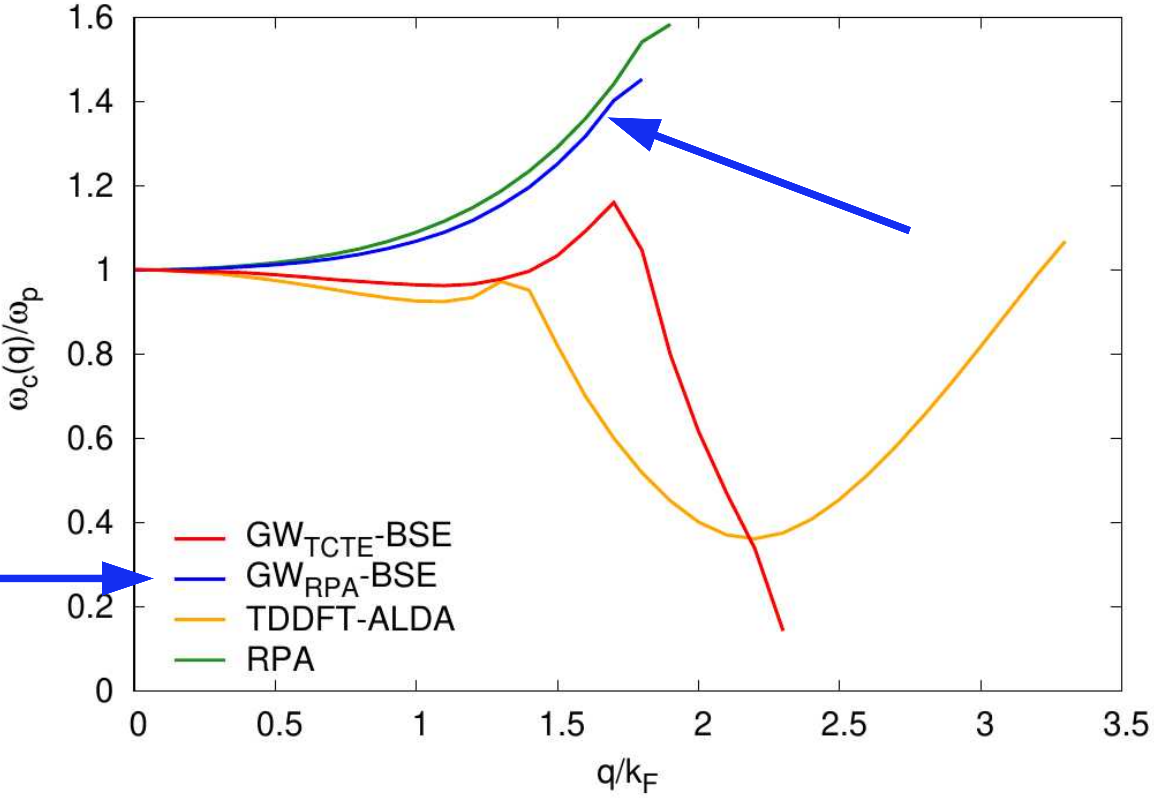
rs=22

Not completely, even with -W in the RPA!

$$
\left.\begin{array}{l}
\epsilon^{\mathrm{in}}(q) \to \Sigma = iGW^{\mathrm{in}} : \quad \text{e-e repulsion} \\
\epsilon^{\mathrm{in}}(q) \to -W^{\mathrm{in}} \;\; : \quad \text{e-h attraction}
\end{array}\right\} \xrightarrow{\mathrm{BSE}} \epsilon^{\mathrm{out}}(q,\omega)
$$

Collective modes:

$$
\mathrm{Re}\,\epsilon^{\mathrm{out}}(q,\omega_c(q)) \;=\; 0
$$



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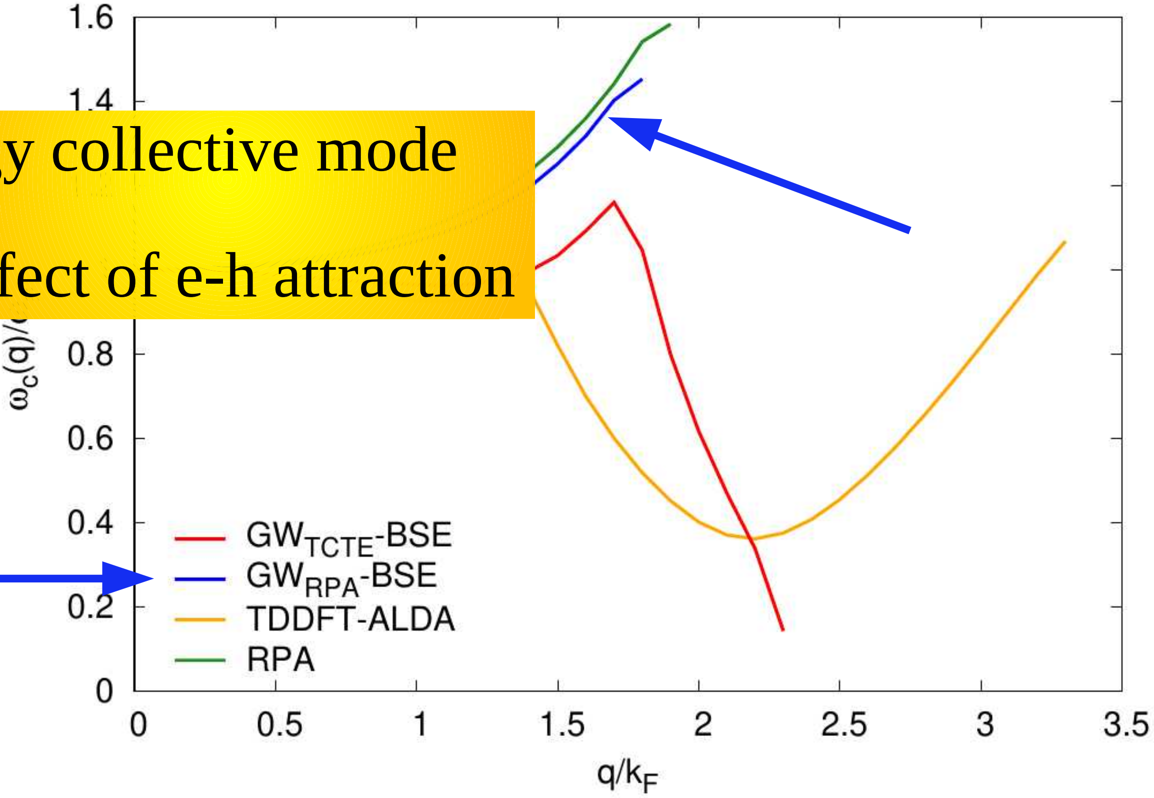
Collective modes

$$\mathrm{Re}\,\epsilon^{\rm out}(q,\omega_c(q)) = 0$$

No low-energy collective mode

Very weak effect of e-h attraction



$$\left.\begin{aligned}\epsilon^{\text{in}}(q) \to \Sigma = iGW^{\text{in}} &: \quad \text{e-e repulsion} \\ \epsilon^{\text{in}}(q) \to -W^{\text{in}} &: \quad \text{e-h attraction}\end{aligned}\right\} \xrightarrow{\text{BSE}} \epsilon^{\text{out}}(q,\omega)$$

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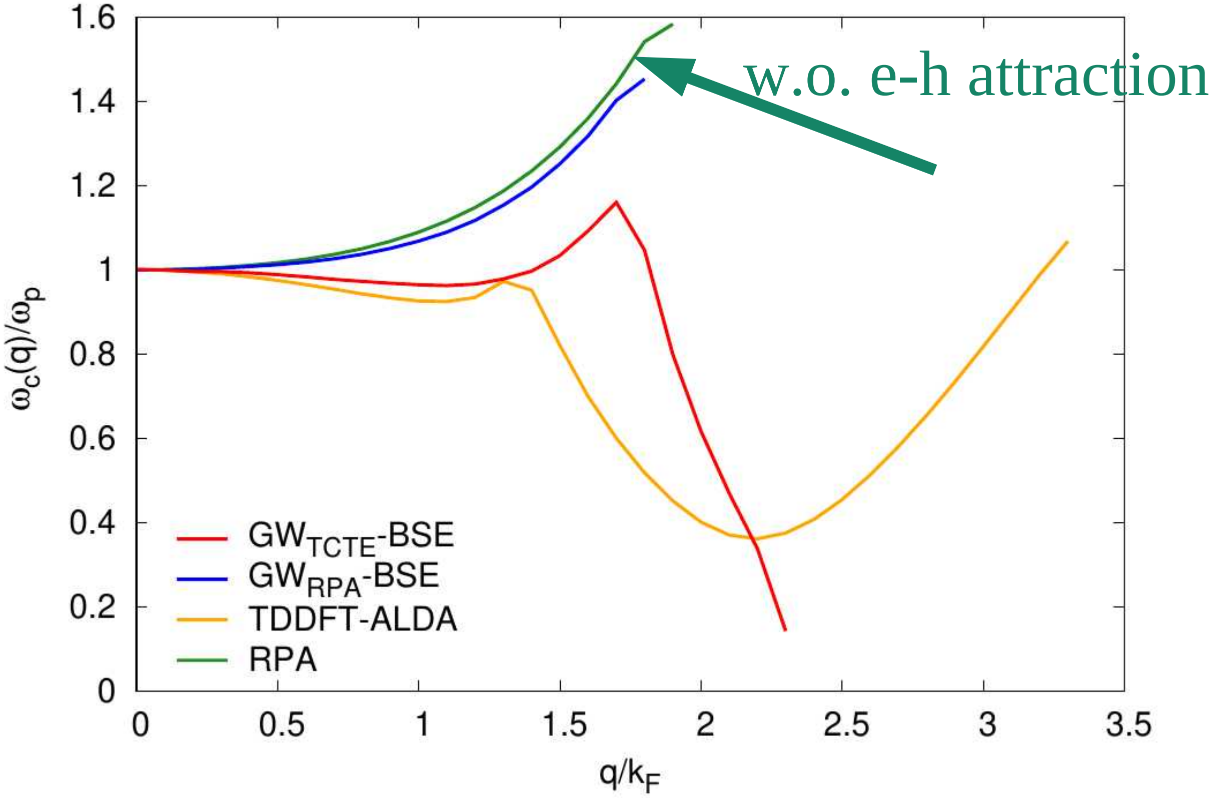
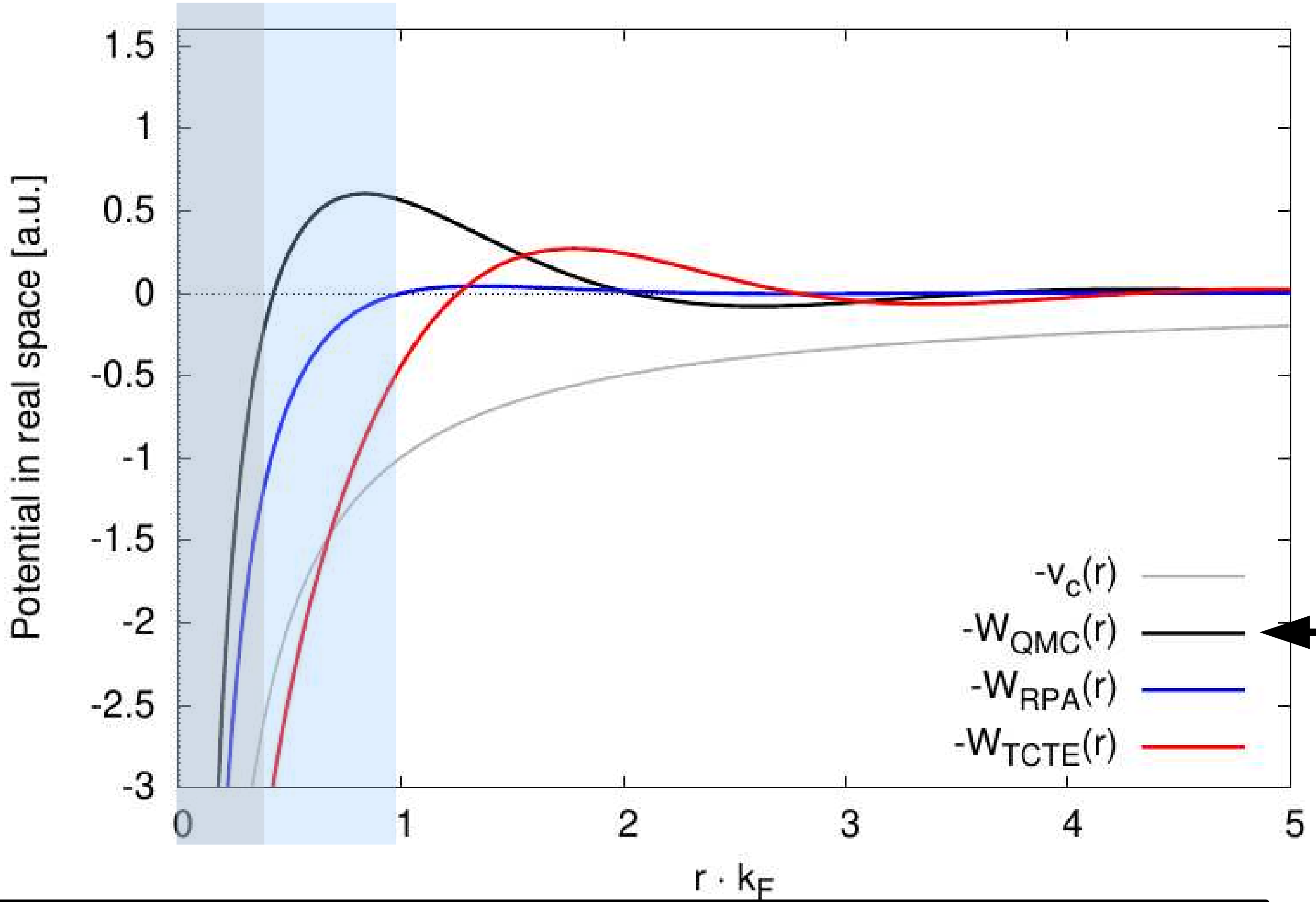


Is this a pb of the RPA W^{in}?

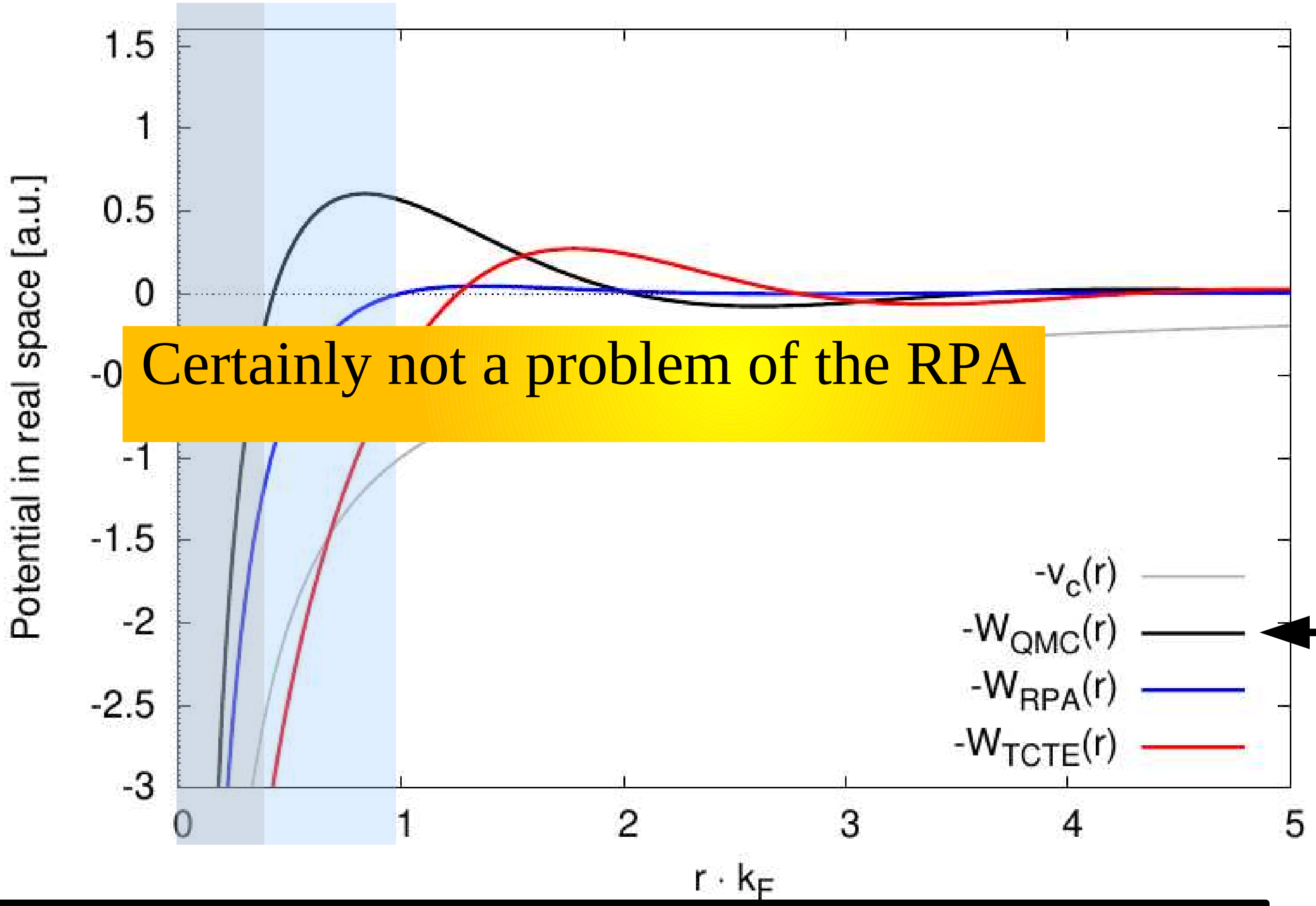


rs=22

Exact (QMC): attractive region even smaller than in the RPA!

Moroni, Ceperley, Senatore, PRL 75, 6 (1995); Corradini, et al. PRB 57, 14569 (1998)

Is this a pb of the RPA W^{in}?



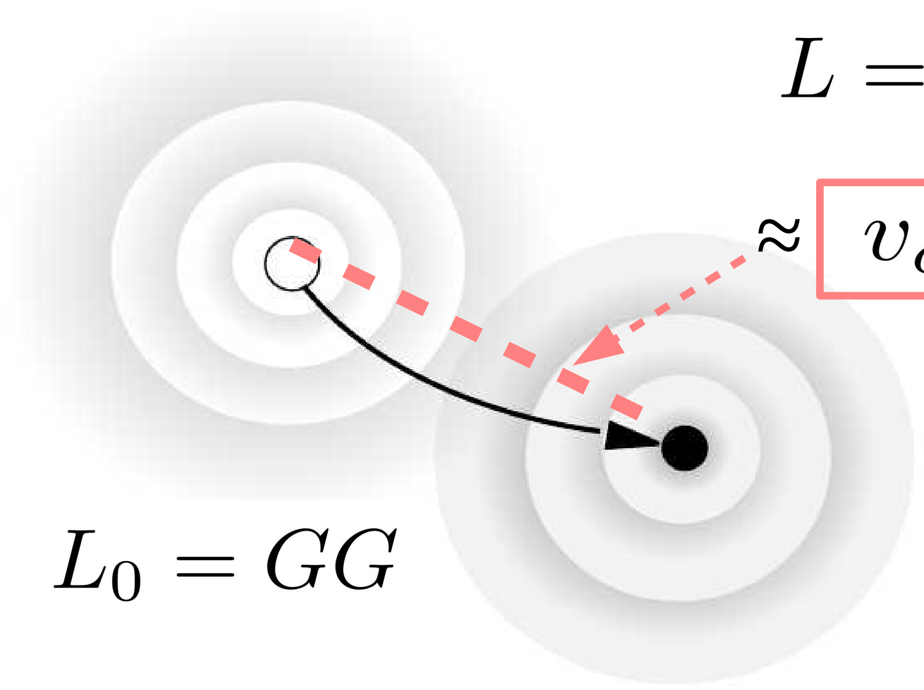
rs=22

Exact (QMC): attractive region even smaller than in the RPA!

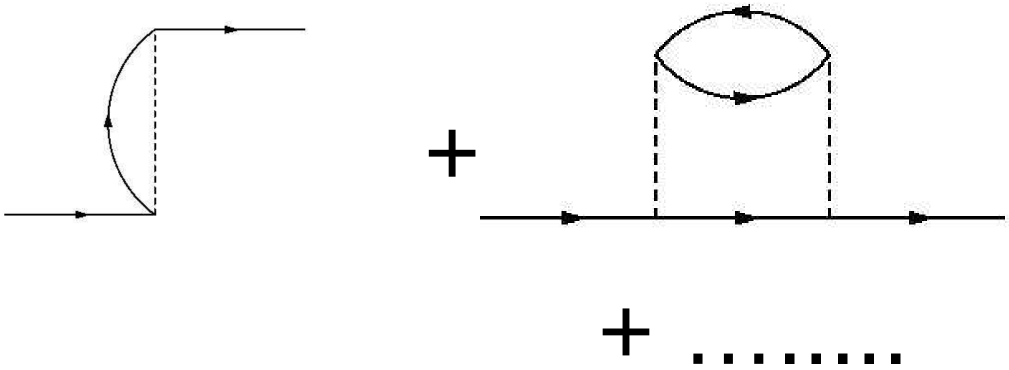
Moroni, Ceperley, Senatore, PRL 75, 6 (1995); Corradini, et al. PRB 57, 14569 (1998)

$$L = L_0 + L_0 \underbrace{\frac{\delta(v_H + \Sigma_{\mathrm{xc}})}{\delta G}}_{\boxed{\text{From GW}}} L$$

$$\approx \boxed{v_c - W}$$

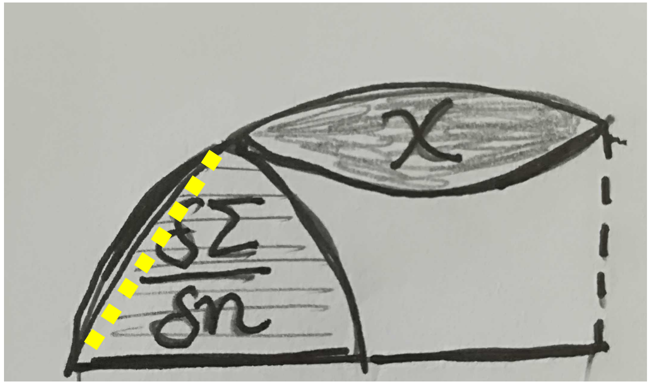


$L_0 = GG$



From TDDFT to vertex corrections beyond GW

"G$\widetilde{\mathrm{W}}$"



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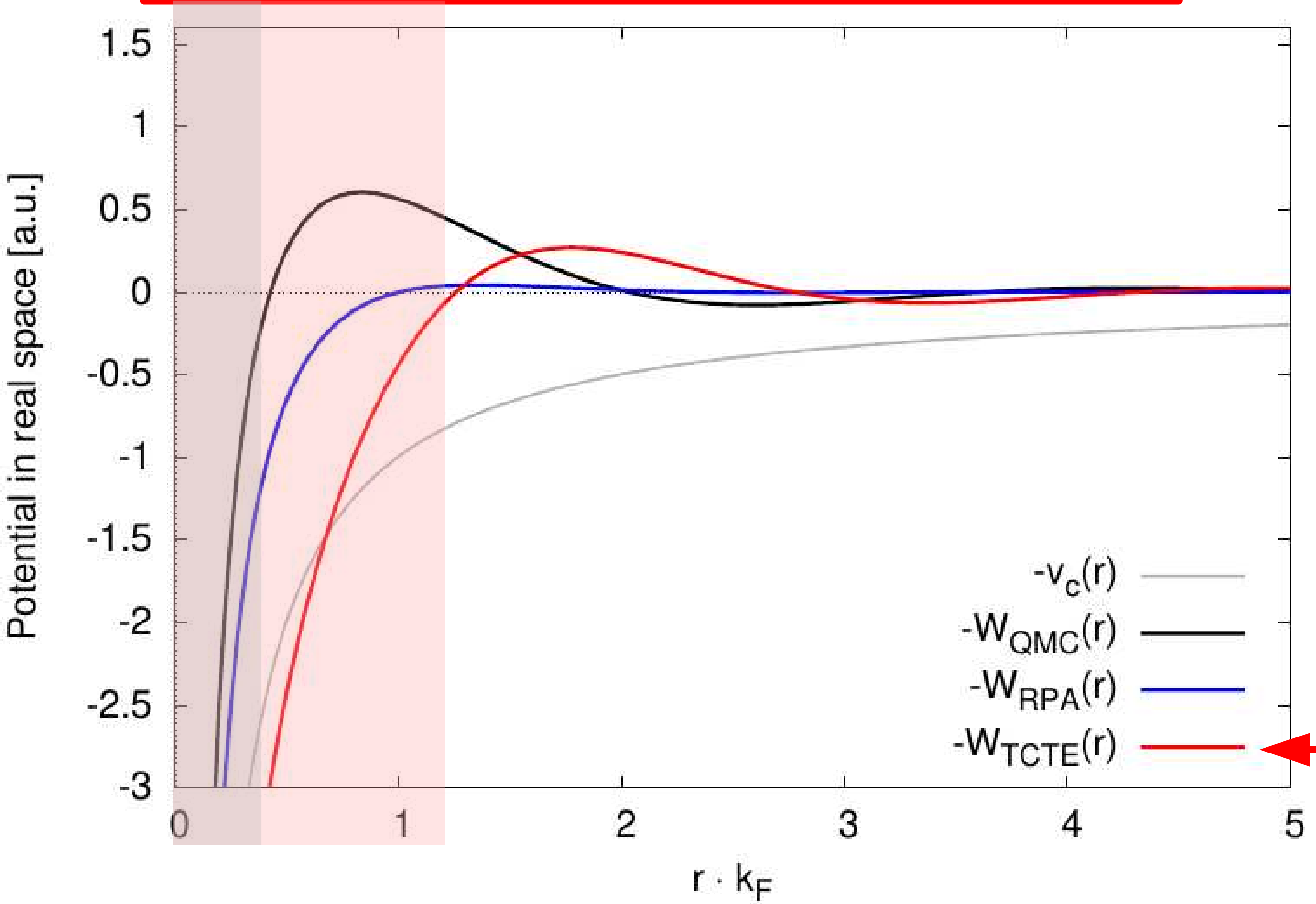
Shishkin, Marsman, and Kresse, PRL 99, 246403 (2007).

$-W^{in}$ should screen fermions: TCTE



rs=22

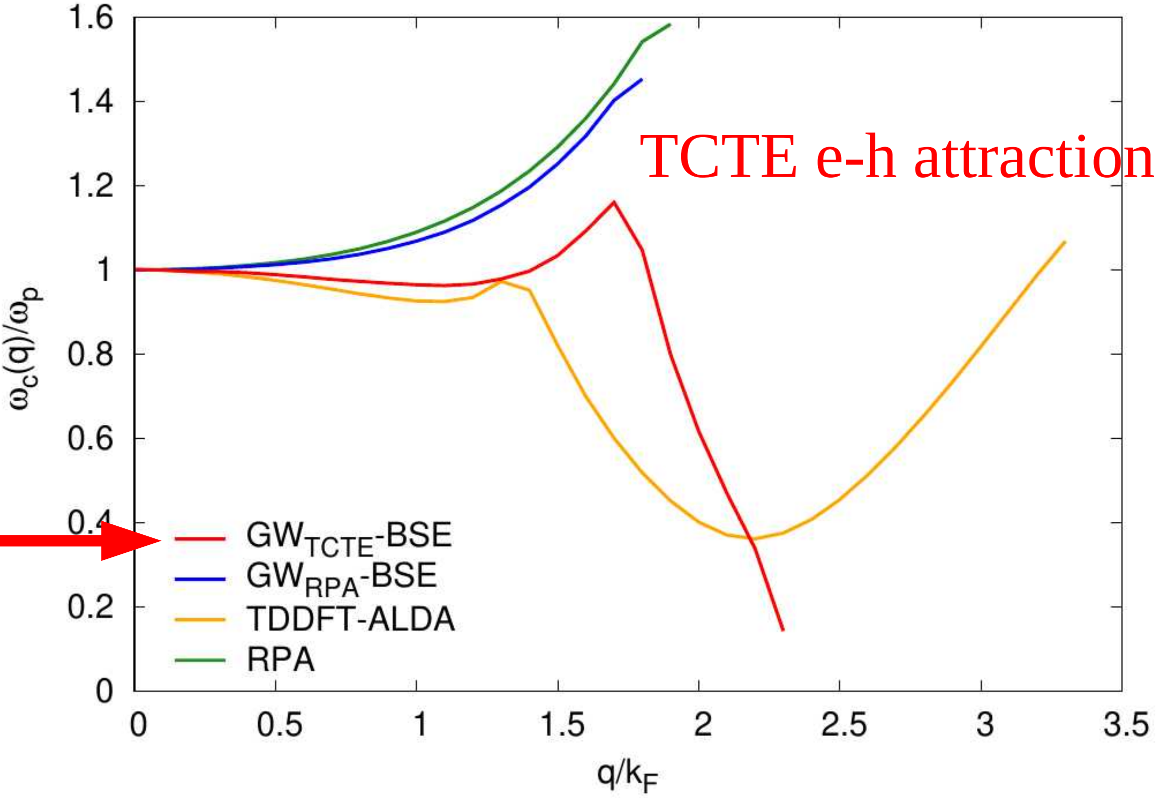
TCTE: attractive region much larger, interaction much stronger

$$\left.\begin{array}{l}\epsilon^{\text{in}}(q) \to \Sigma = iGW^{\text{in}} : \quad \text{e-e repulsion} \\ \epsilon^{\text{in}}(q) \to -W^{\text{in}} \ : \quad \text{e-h attraction}\end{array}\right\} \xrightarrow{\text{BSE}} \epsilon^{\text{out}}(q,\omega)$$

Collective modes:

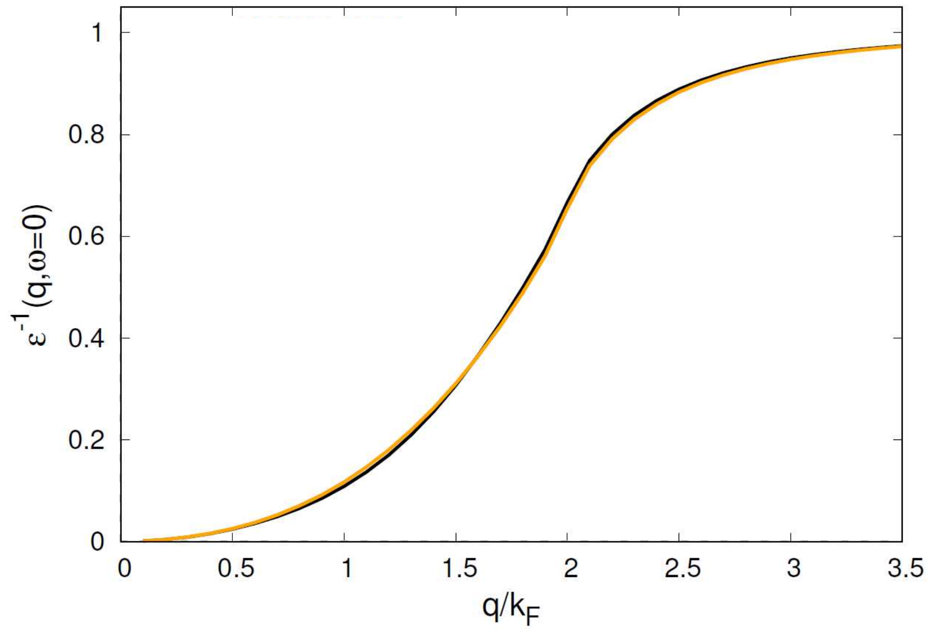
$$\mathrm{Re}\,\epsilon^{\text{out}}(q,\omega_c(q)) = 0$$

TCTE e-h attraction



QMC

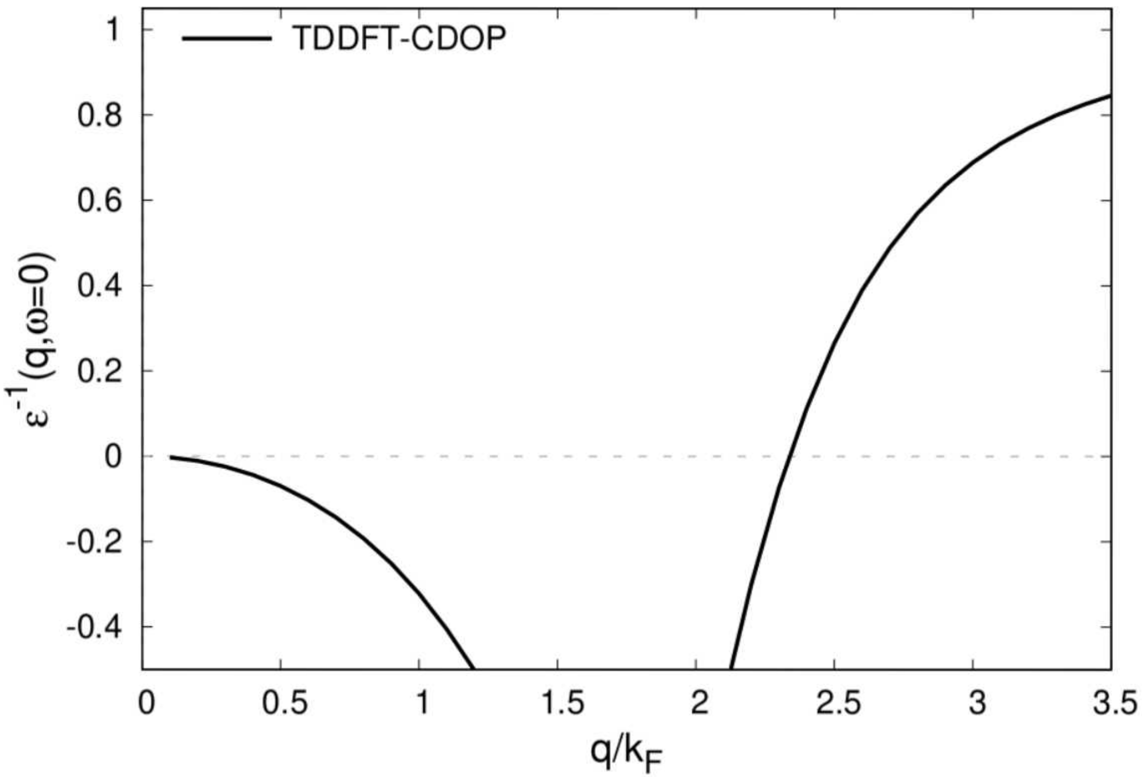
M. Corradini, et al., PRB 57, 14569 (1998)
S. Moroni, D. M. Ceperley, and G. Senatore,
PRL 75, 6 (1995)



HEG, rs=4

Static screening

rs=22



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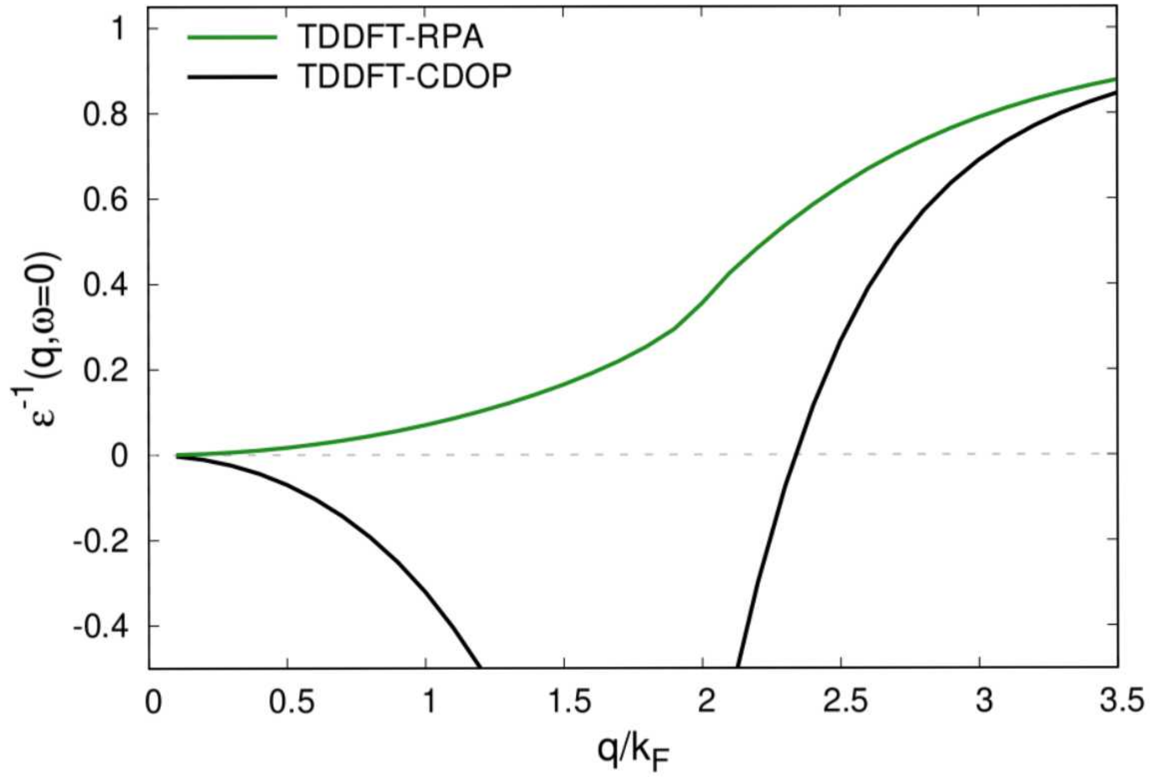

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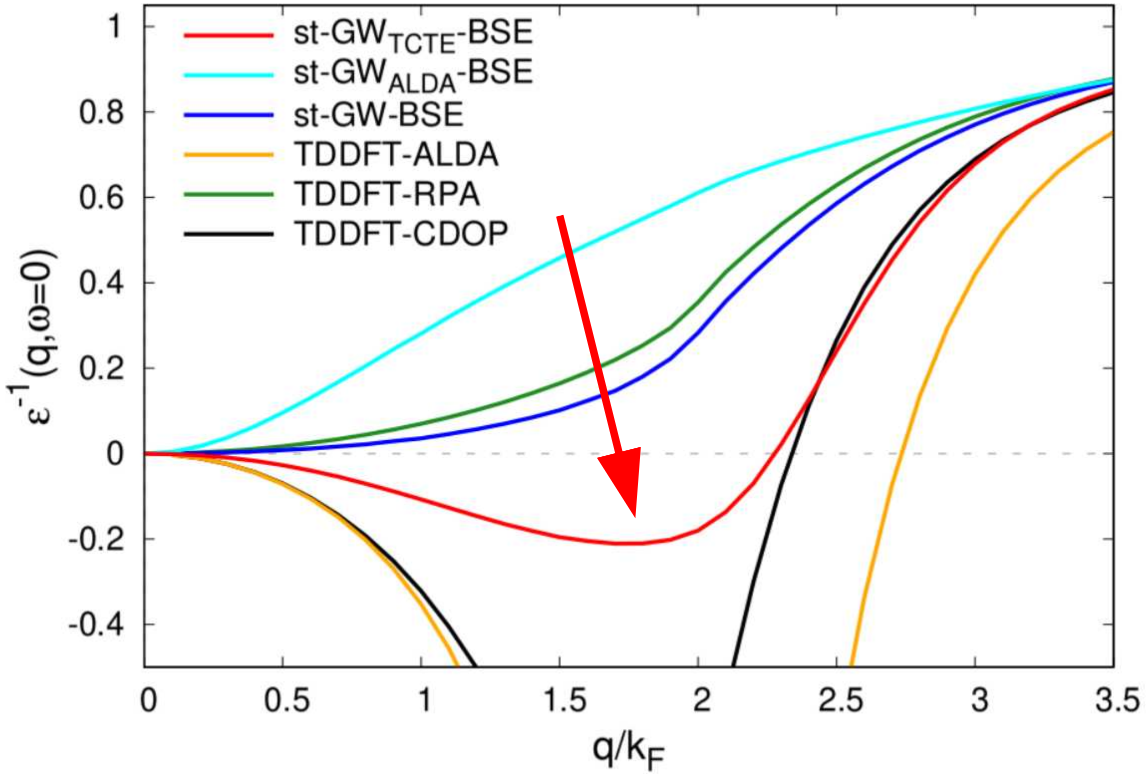

See also:
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K. Chen and K. Haule, Nature Communications 10, 3725 (2019)
T. Dornheim, S. Groth, and M. Bonitz, Physics Reports 744, 1 (2018)
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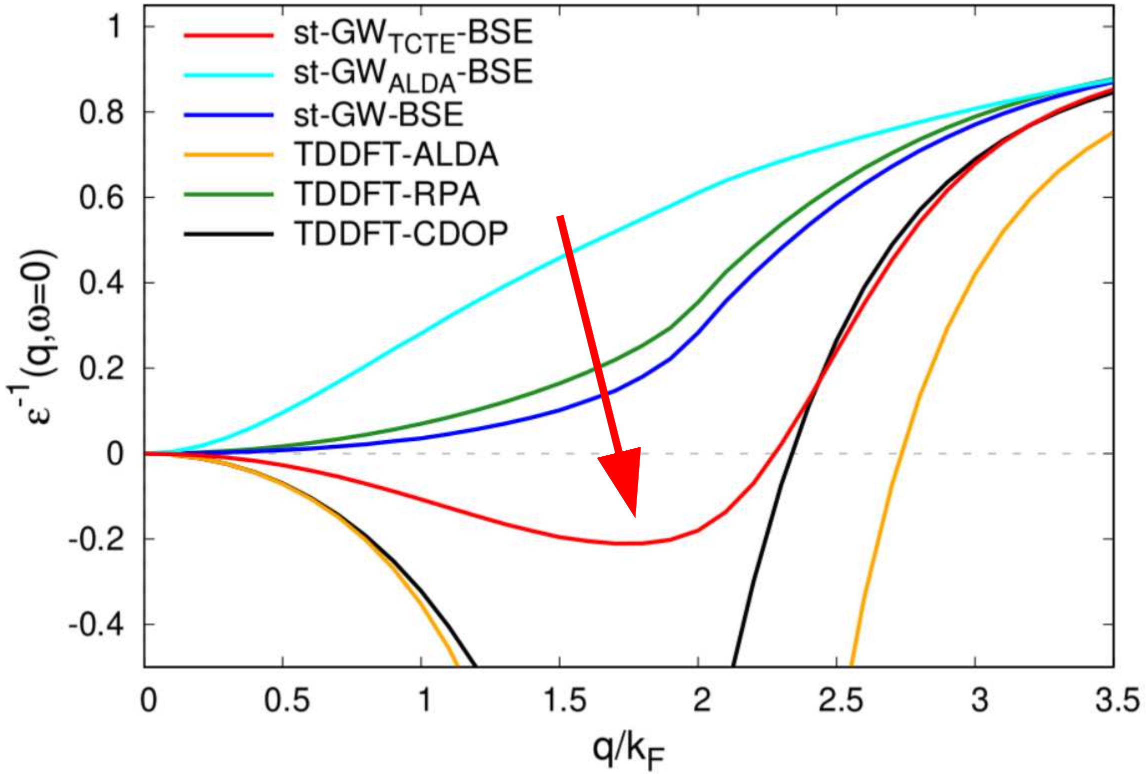
S. Groth, T. Dornheim, and J. Vorberger, Phys. Rev. B 99, 235122 (2019)

Koskelo, Reining, Gatti, Phys. Rev. Lett. 134, 046402 (2025)



Low-energy modes
negative plasmon dispersion
and negative static screening
in the low-density HEG

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T. Dornheim, S. Groth, and M. Bonitz, Physics Reports 744, 1 (2018)
T. Dornheim, S. Groth, J. Vorberger, and M. Bonitz, Phys. Rev. Lett. 121, 255001 (2018)
S. Groth, T. Dornheim, and J. Vorberger, Phys. Rev. B 99, 235122 (2019)

Koskelo, Reining, Gatti, Phys. Rev. Lett. 134, 046402 (2025)

The electron-hole BSE as 2-particle problem

$$H_{\mathrm{exc}}\Psi_\lambda(\mathbf{r}_h,\mathbf{r}_e) = E_\lambda \Psi_\lambda(\mathbf{r}_h,\mathbf{r}_e)$$

Intensities

Excitation energies

$$\left.\begin{array}{l} \epsilon^{\mathrm{in}}(q,\omega) \to \Sigma = iGW^{\mathrm{in}} : \quad \text{e-e repulsion} \\ \epsilon^{\mathrm{in}}(q,\omega=0) \to -W^{\mathrm{in}} : \quad \text{e-h attraction} \end{array}\right\} \xrightarrow{\mathrm{BSE}} \epsilon^{\mathrm{out}}(q,\omega)$$

$$v_{\text{tot}}(\omega) = \epsilon^{-1}(\omega) v_{\text{ext}}(\omega)$$

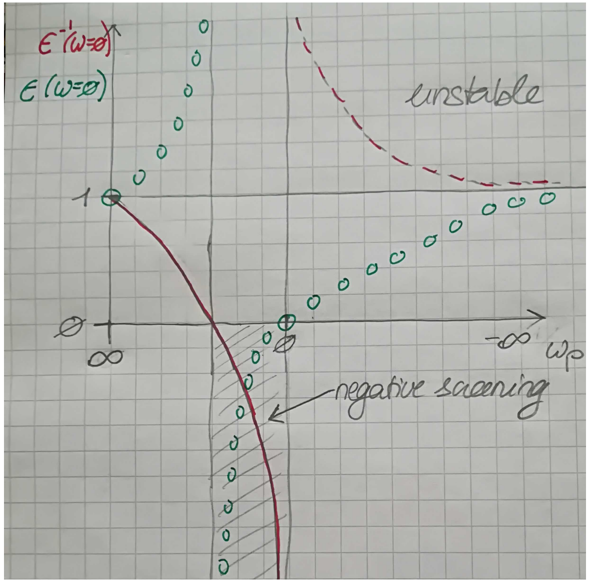
Is a ghost important?

$$\epsilon^{-1}(\omega) = 1 + v_c \chi(\omega)$$

$$\chi(\omega) = a \frac{2\omega_p}{\omega^2 - \omega_p^2} \qquad \epsilon^{-1}(\omega) = 1 + v_c \, a \frac{2\omega_p}{\omega^2 - \omega_p^2}$$

$$\epsilon^{-1}(\omega = 0) = 1 - \frac{2 v_c \, a}{\omega_p} \qquad < 0 \text{ for } \omega_p < 2 a v_c$$

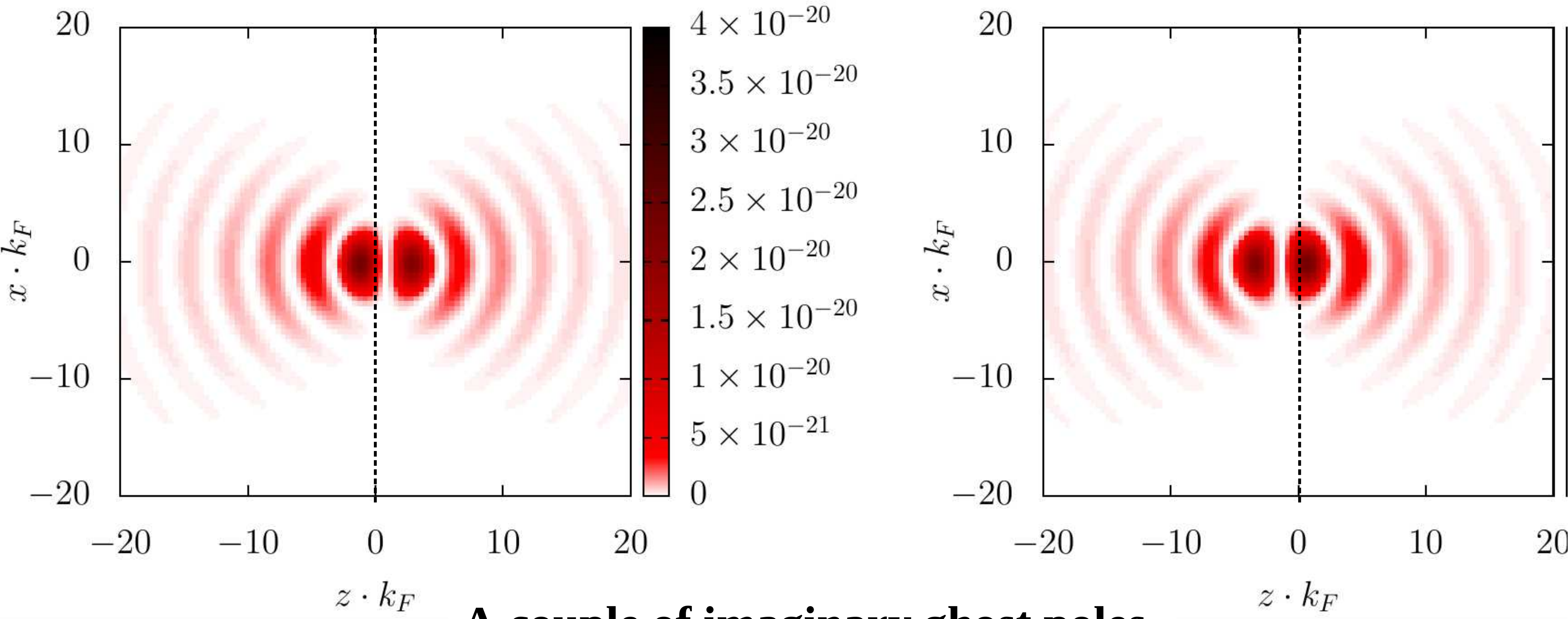
$$\epsilon^{-1}(\omega = 0) < 0 \quad \rightarrow \quad \epsilon(\omega = 0) < 0$$



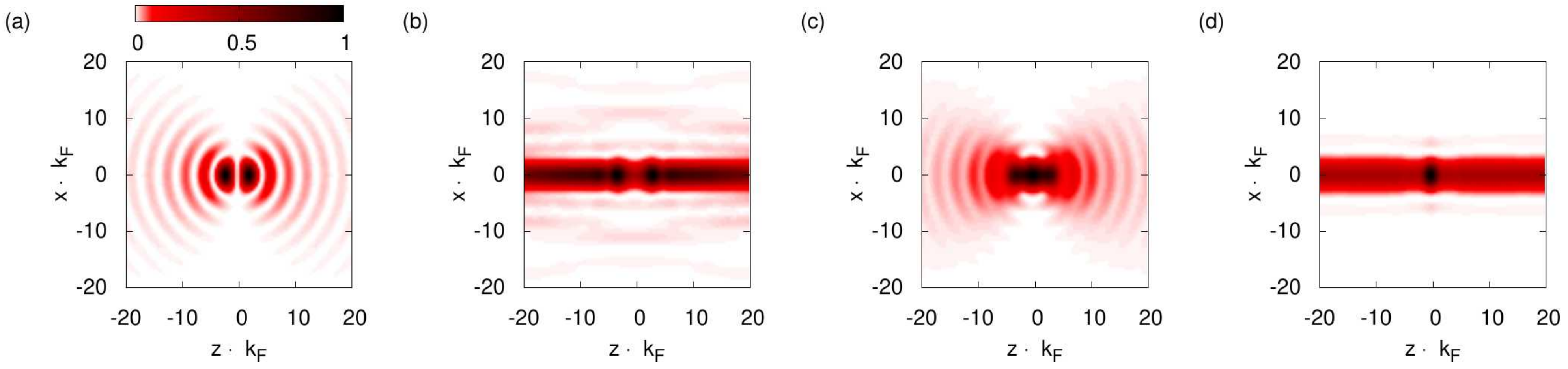
$$\epsilon(\omega) = \frac{\omega^2 - \omega_p^2}{\omega^2 - \omega_p^2 + 2 a v_c \omega_p}$$

$$\epsilon = 1 - v_c P$$

Complex Pole at $\omega = \pm\sqrt{\omega_p^2 - 2 a v_c \omega_p}$



A couple of imaginary ghost poles



Plasmon

Low-energy mode

Ghost mode

Low-energy mode in ALDA

Poles of χ

$q=2k_F$ along z

Ghost and low energy modes in the low-density HEG

→ Accessible via BSE with vertex corrections

→ Effect of weakening of screening at short distances

→ Short-time effects also to be explored

Koskelo, Reining, Gatti, Phys. Rev. Lett. 134, 046402 (2025) Editor's choice

BSE+vertex: highly anisotropic e-h correlation

Combining many-body perturbation theory and TDDFT: getting the best of both worlds

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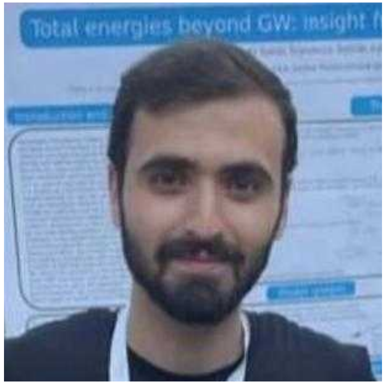
* fxc from the Bethe-Salpeter equation of MBPT

* vertex corrections beyond GW from TDDFT



Abdallah El Sahili

→ Our today's research:

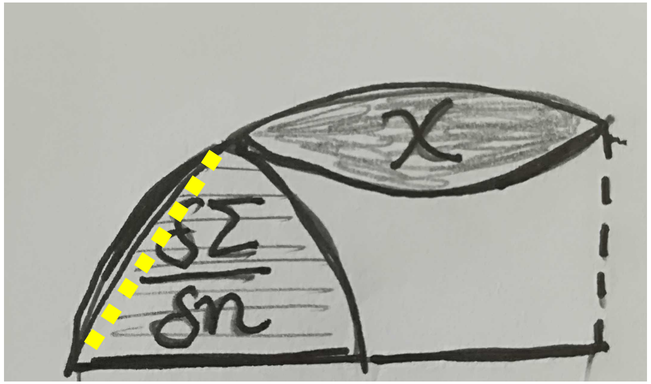
* fxc approx. vertex corrections: exotic excitations in the HEG

* How wrong are fxc approx. vertex corrections *in principle?*

→ A central quantity: Σ[n]

An old idea for the correlation self-energy:

“G$\tilde{W}$”



$= v_c + f_{xc}$

Beyond GW, approximate vertex from TDDFT: $i\dfrac{\delta\Sigma_{xc}}{\delta G} \rightarrow \dfrac{\delta v_{xc}}{\delta n} = f_{xc}$

Overhauser, PRB 3, 1888 (1971); Petrillo and Sacchetti, PRB 38, 3834 (1988);
Mahan and Sernelius, PRL. 62, 2718 (1989); Hybertsen and Louie, PRB 34, 5390 (1986);
Del Sole, Reining, and Godby, PRB 49, 8024 (1994); Hindgren and Almbladh, PRB 56, 12832 (1997);
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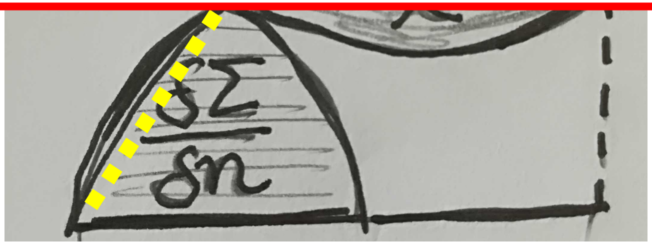
Shishkin, Marsman, and Kresse, PRL 99, 246403 (2007).

An old idea for the correlation self-energy:

This will have errors from the procedure

and from approx. of f_{xc}

$= v_c + f_{\mathrm{xc}}$



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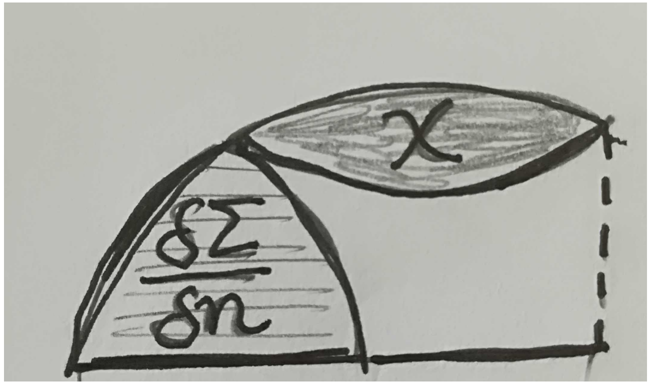
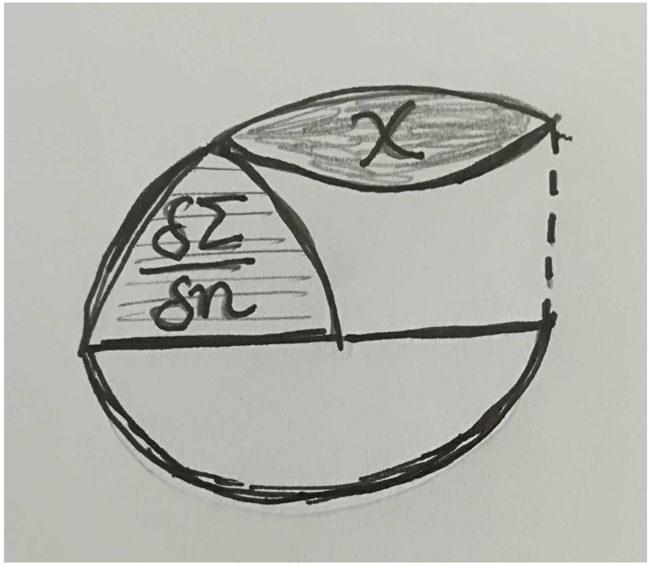
Correlation self-energy



Correlation energy (no kinetic contribution)



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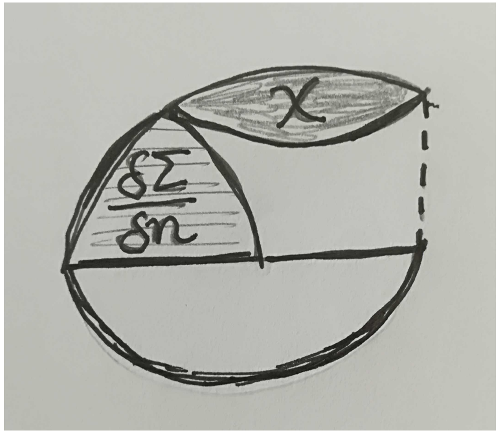
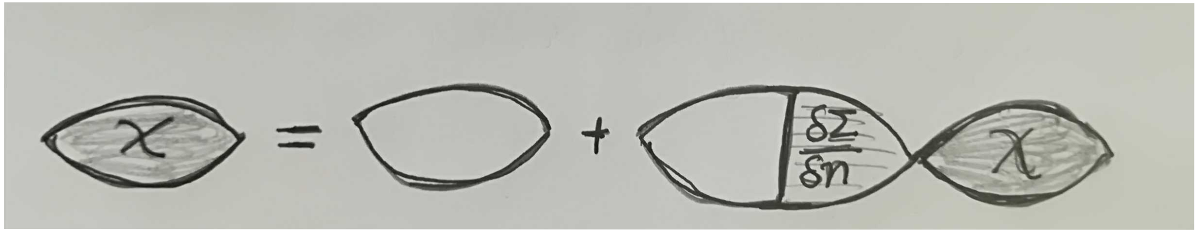
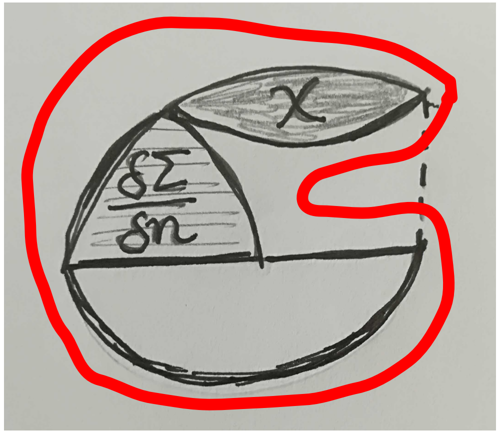
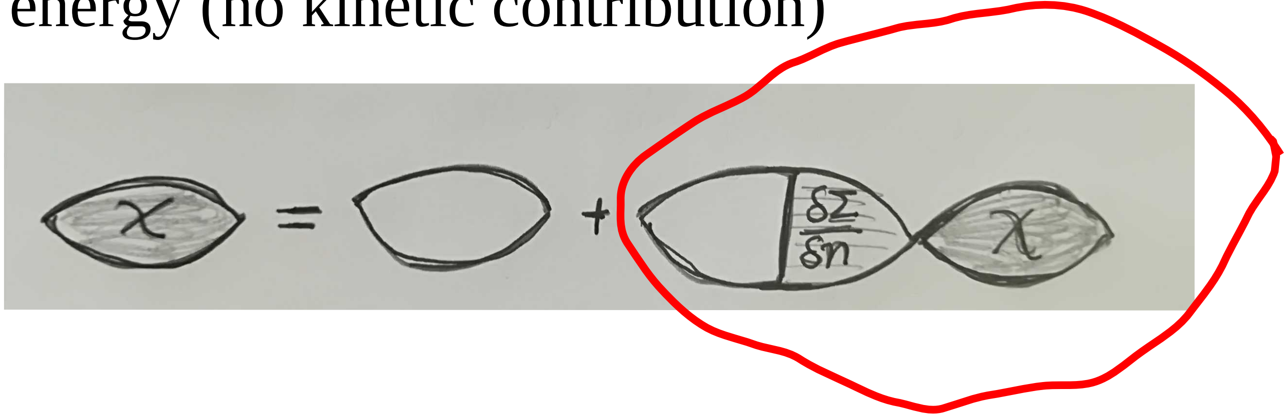




mb effective “TDDFT”
(→ NQ kernel etc)

Correlation energy (no kinetic contribution)





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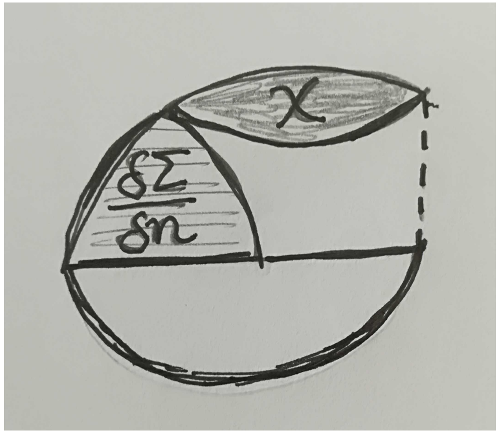
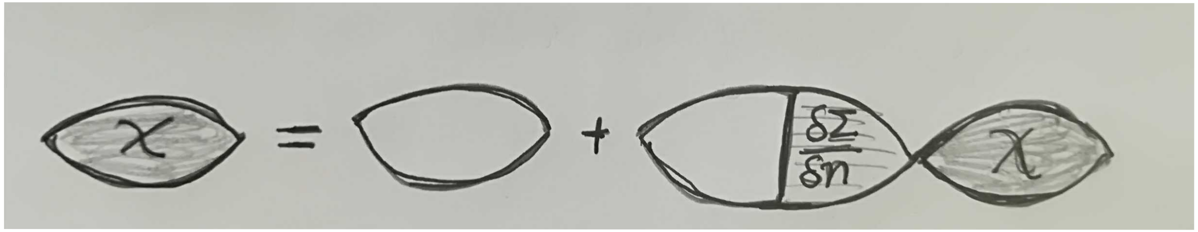
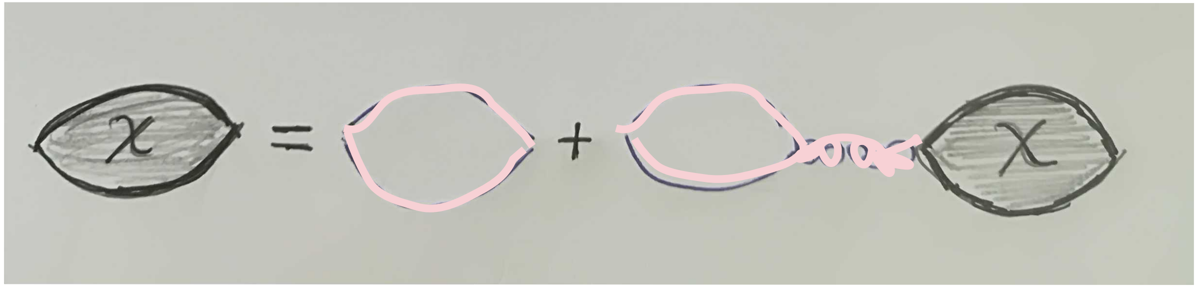




Same response fct from true TDDFT



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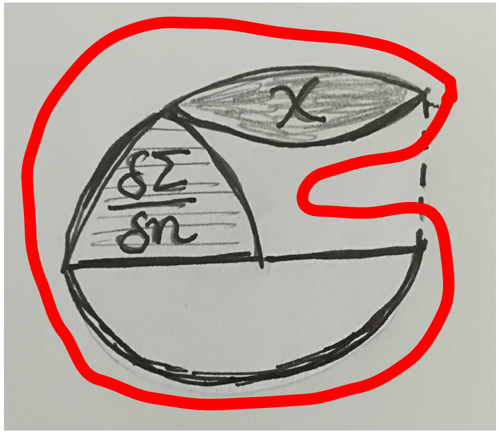

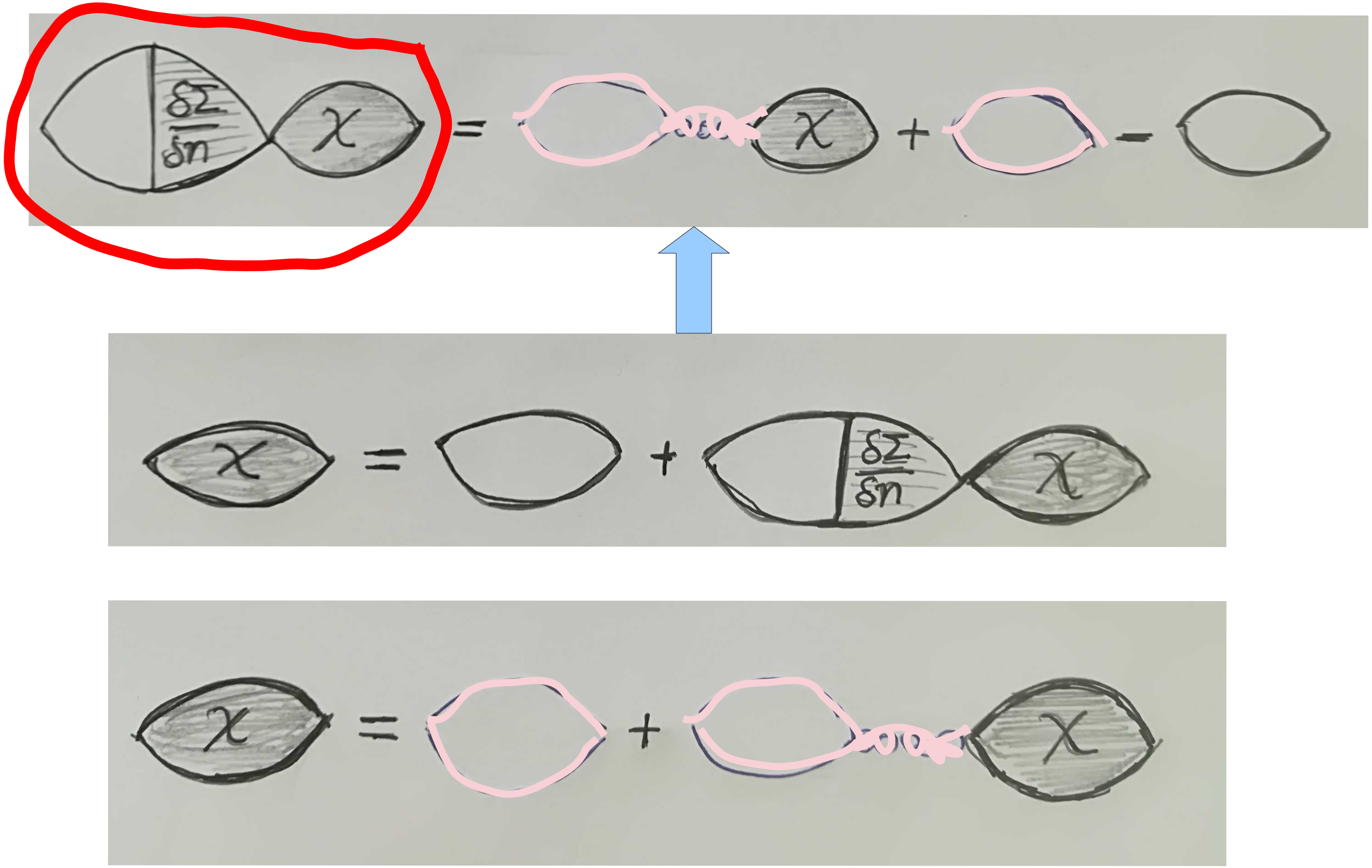

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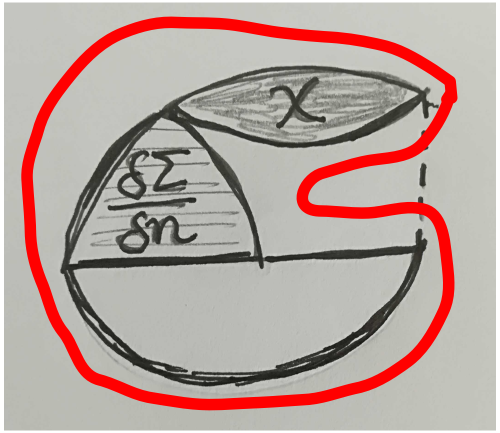

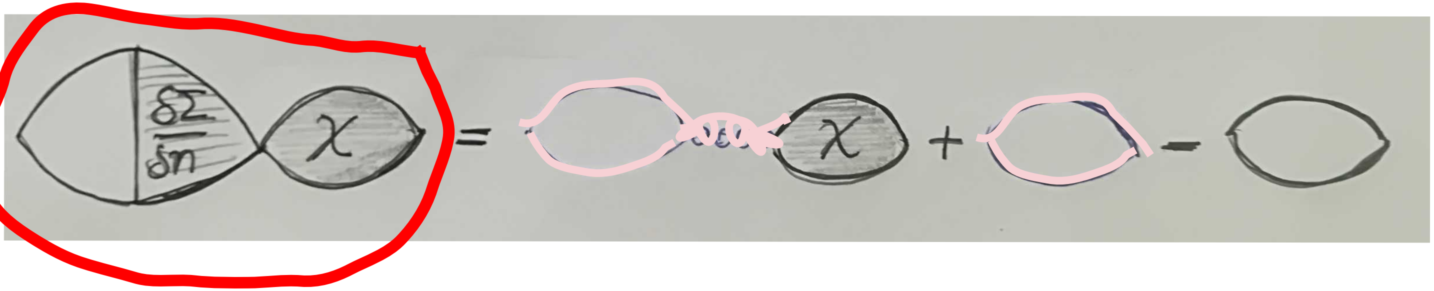

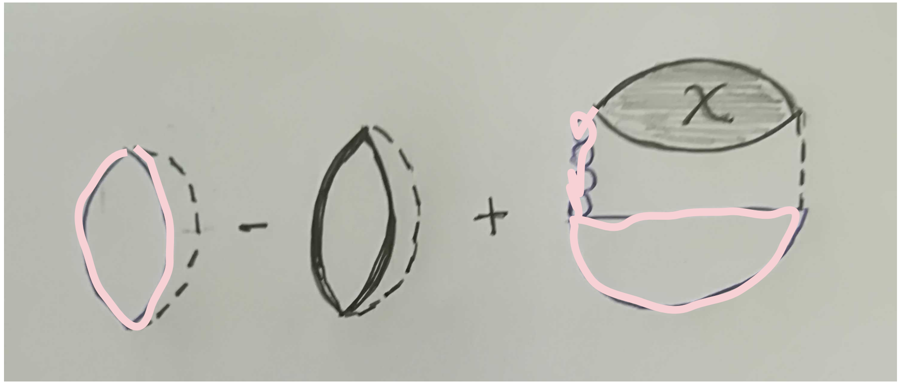

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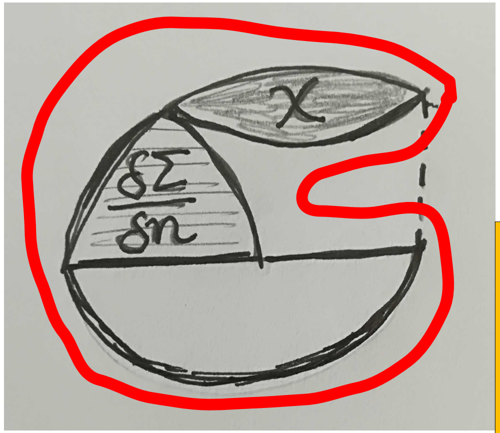
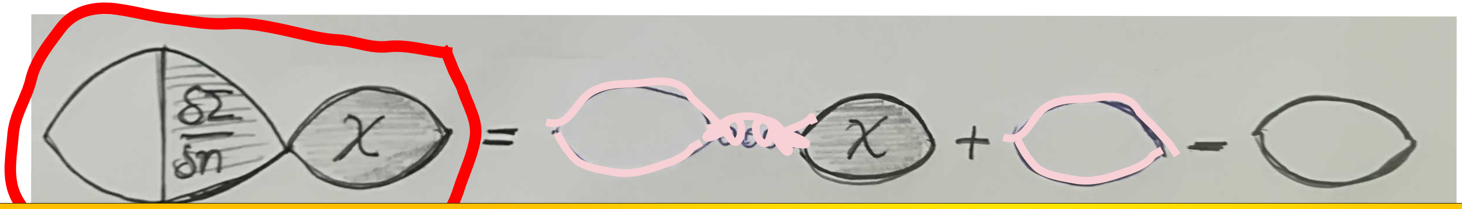
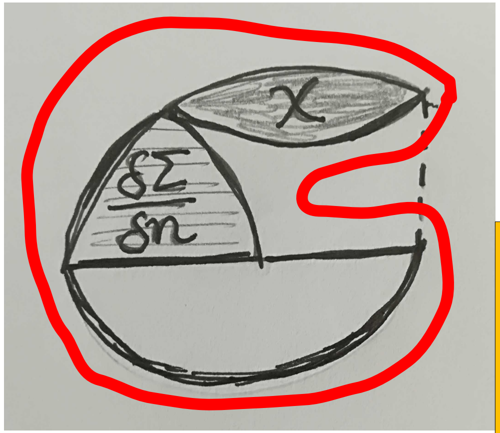
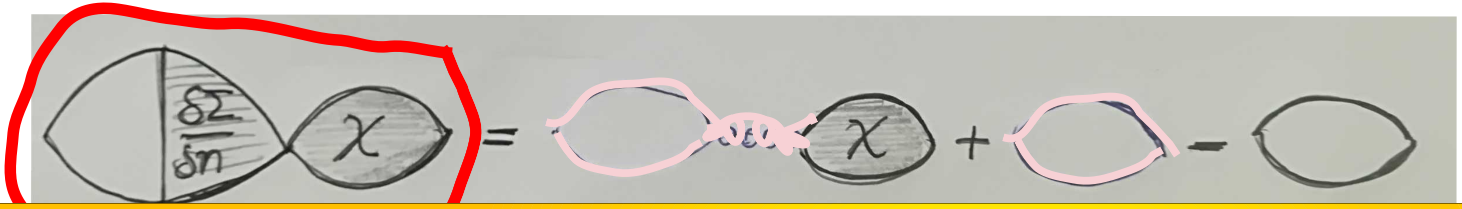




The (approximate!!!) $G\tilde{W}$ self-energy together with an xchange correction yields the exact correlation energy

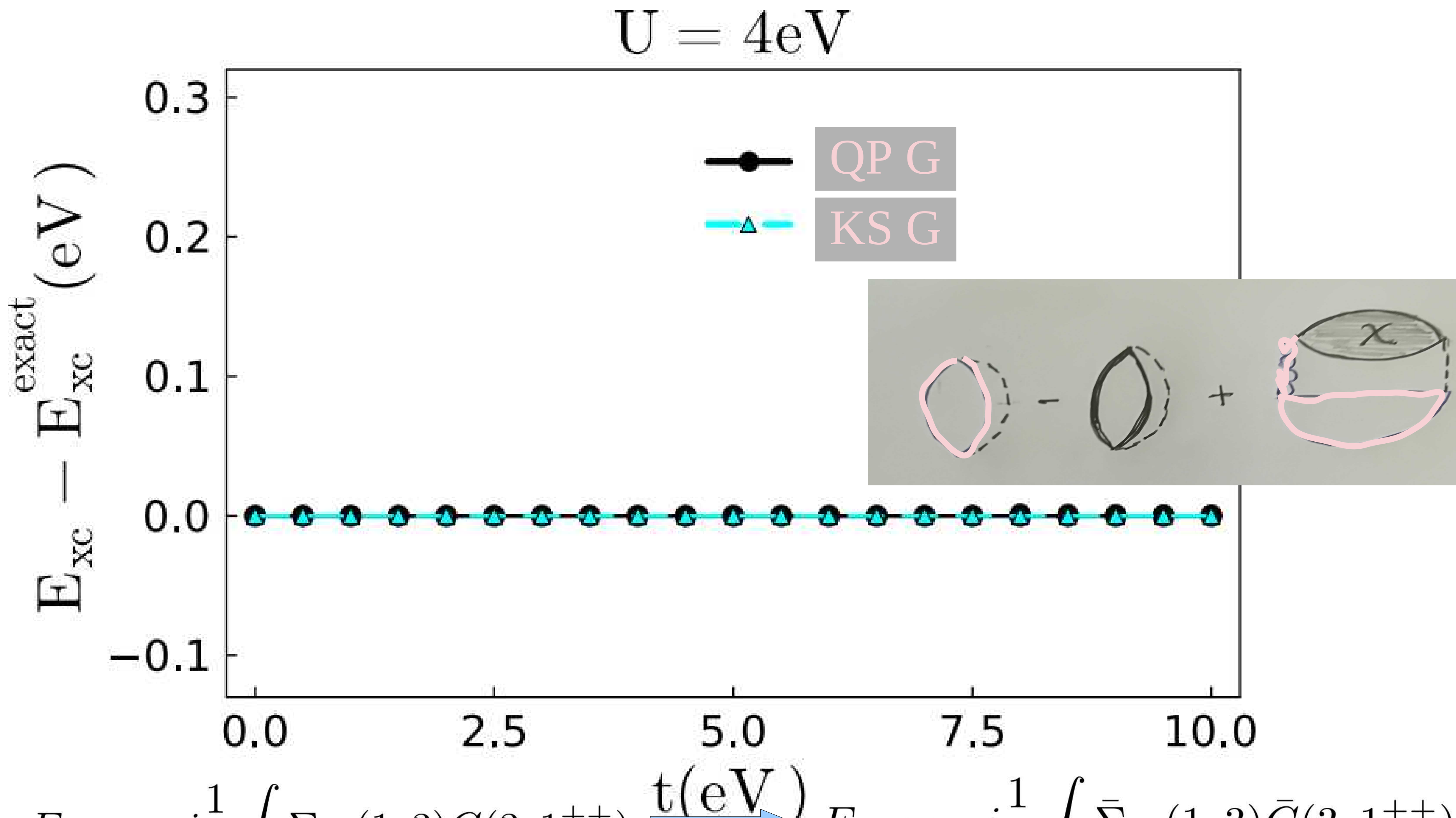
Correlation energy (no kinetic contribution)



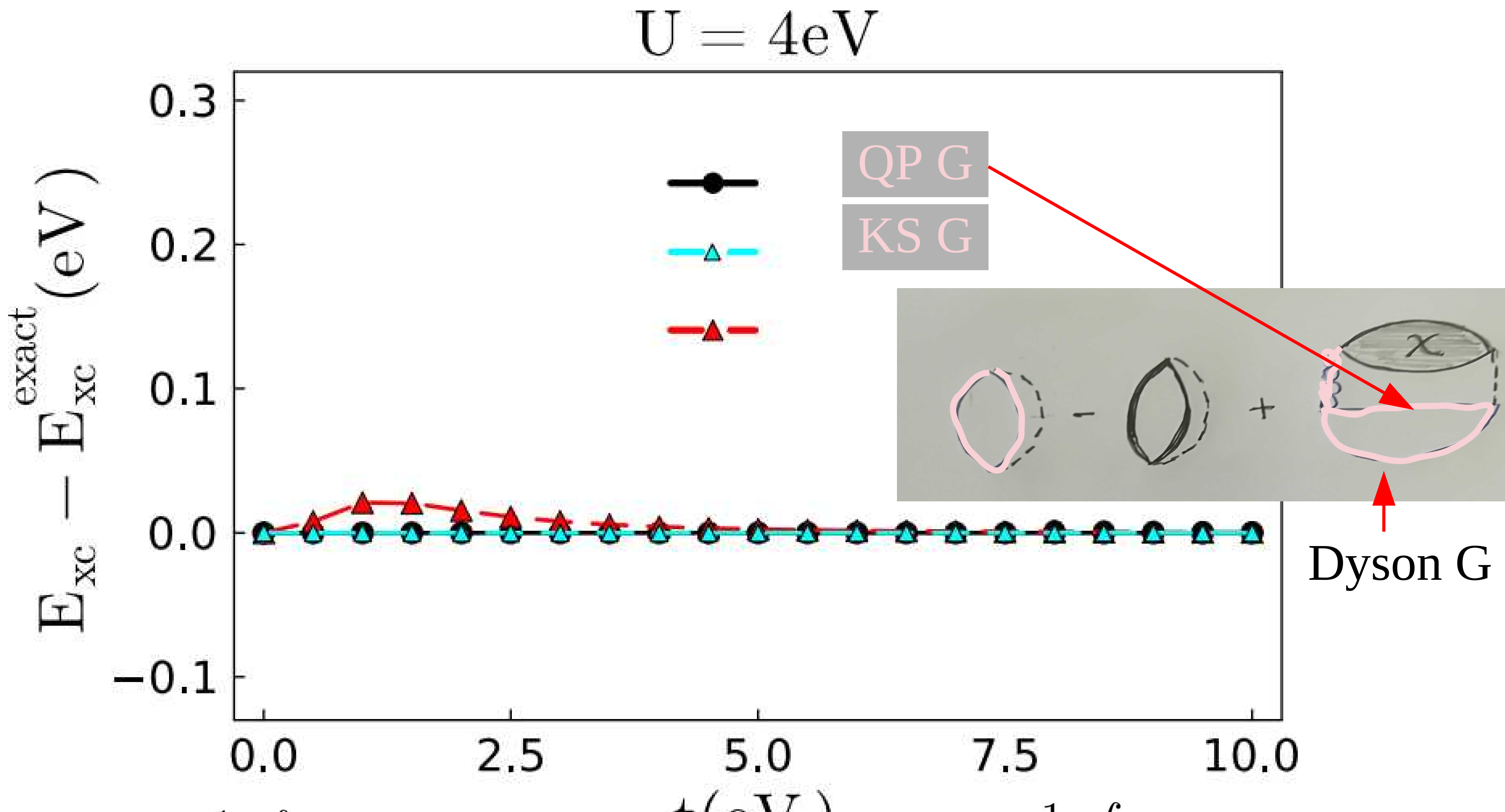


The (approximate!!!) G$\tilde{W}$ self-energy together with an xchange correction yields the exact correlation energy

Of course, not the exact spectral function



$$E_{\mathrm{xc}} = -i\frac{1}{2}\int \Sigma_{\mathrm{xc}}(1,3)G(3,1^{++}) \longrightarrow E_{\mathrm{xc}} = -i\frac{1}{2}\int \bar{\Sigma}_{\mathrm{xc}}(1,3)\bar{G}(3,1^{++})$$



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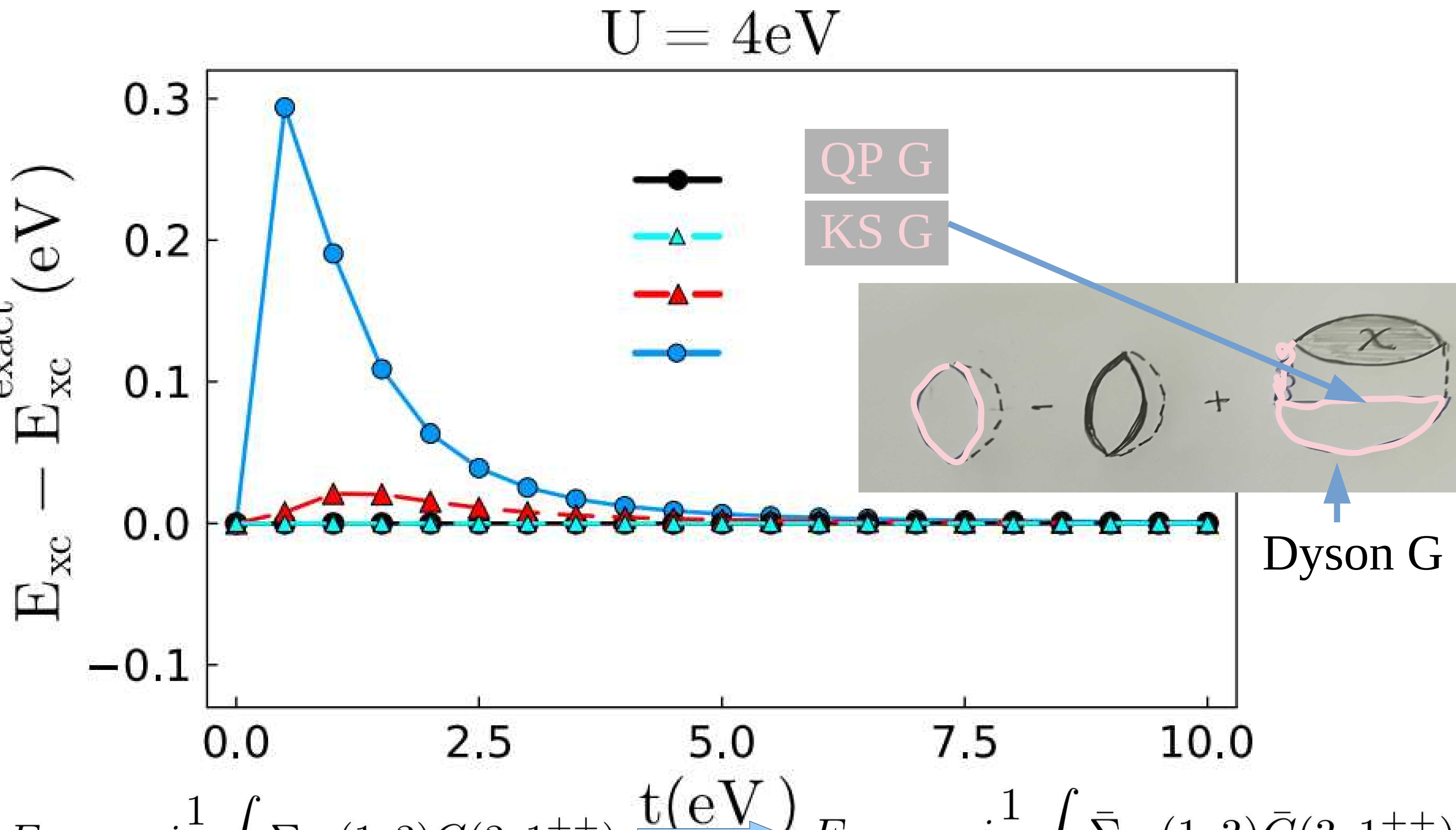

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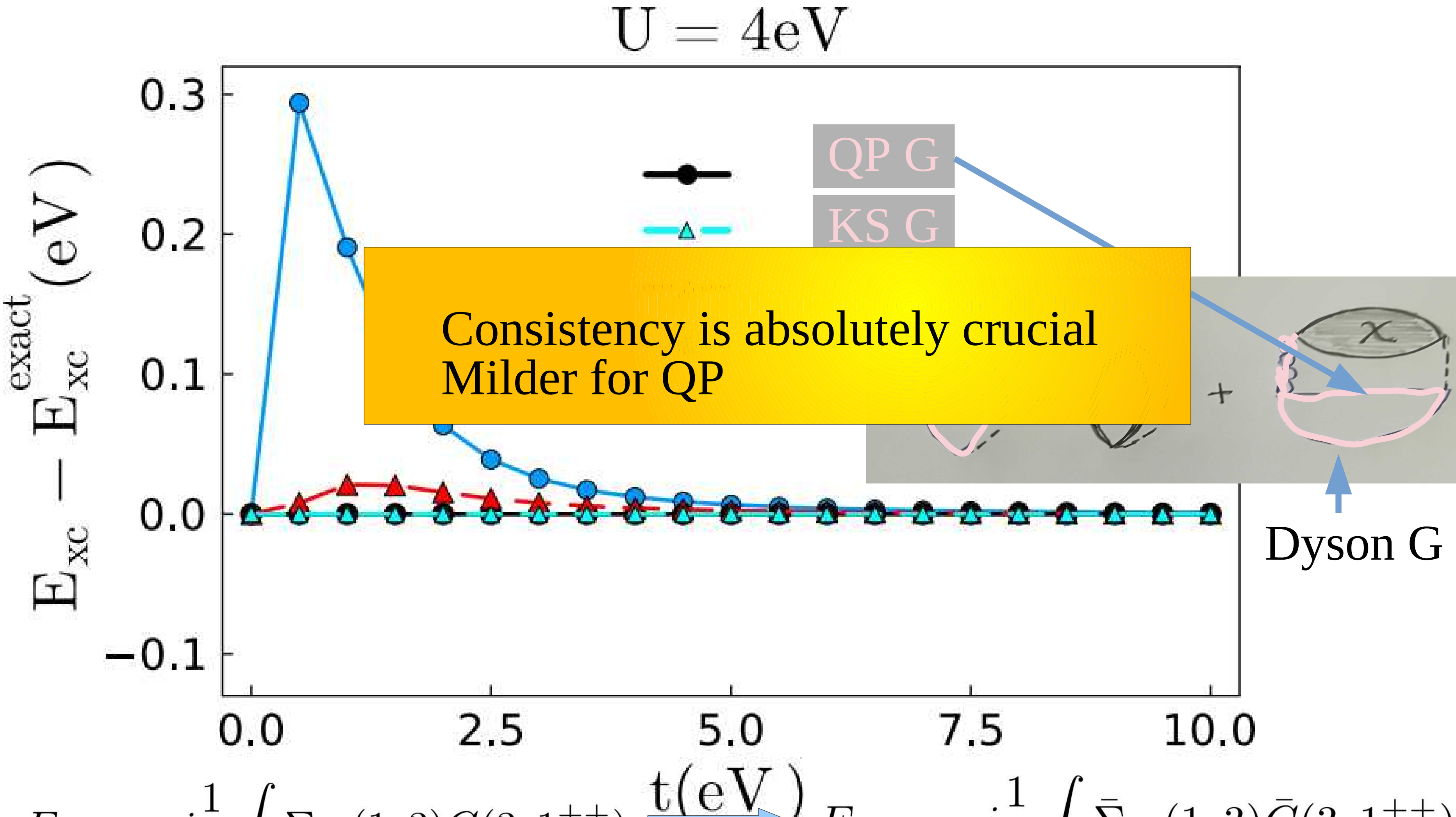
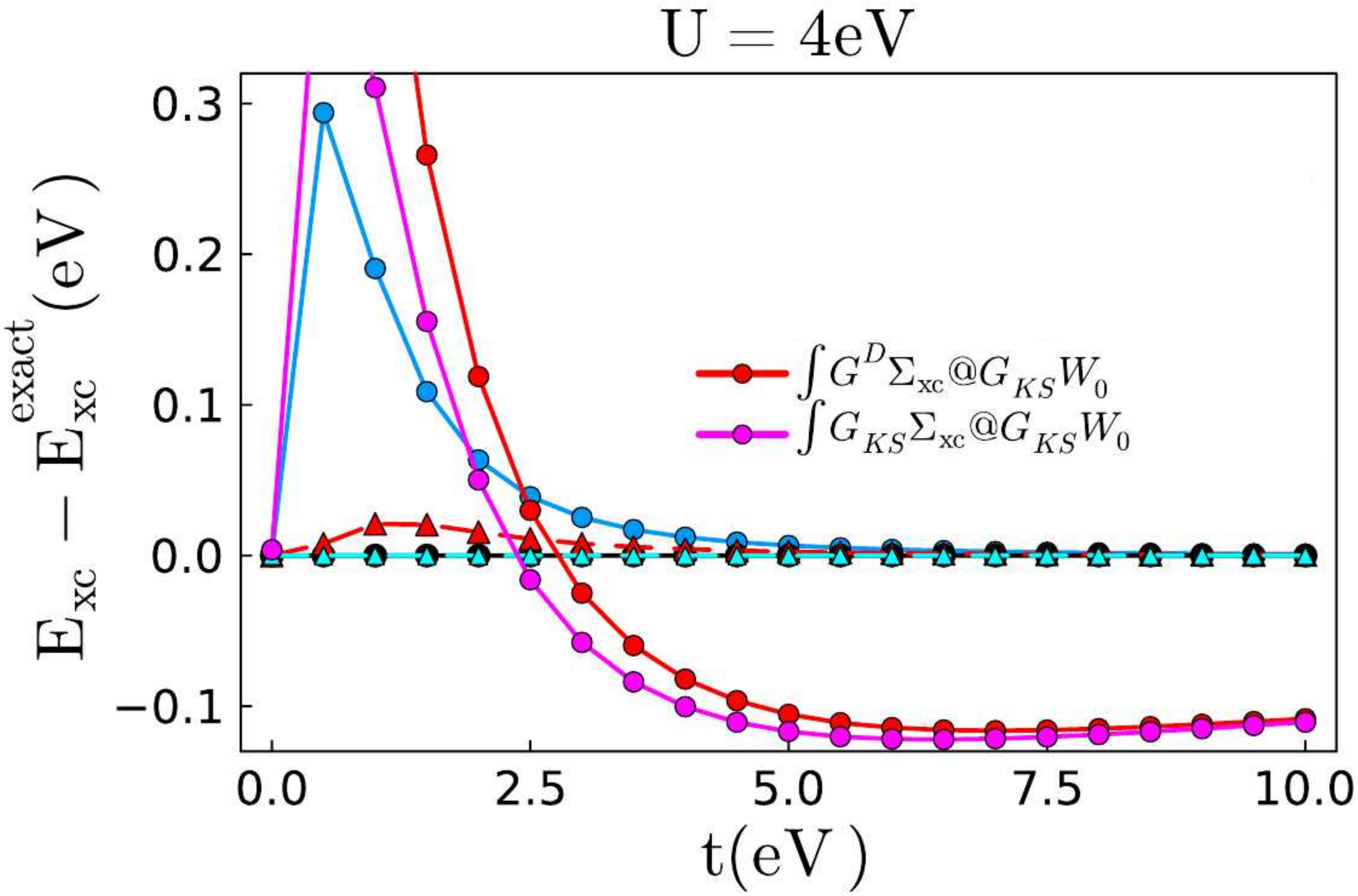


Consistency is absolutely crucial
Milder for QP

Dyson G

$$E_{\mathrm{xc}} = -i\frac{1}{2}\int \Sigma_{\mathrm{xc}}(1,3)G(3,1^{++}) \rightarrow E_{\mathrm{xc}} = -i\frac{1}{2}\int \bar{\Sigma}_{\mathrm{xc}}(1,3)\bar{G}(3,1^{++})$$

Error much reduced wrt GW



The $G\widetilde{W}$ approx. self-energies yield the exact xc energy
if the expression is evaluated consistently

……. but not the exact G nor the exact density matrix nor kinetic energy!

→ When the TDDFT input is exact, QPs are quite ok while sat.s are bad

→ The adiabatic approximation to the xc kernel does ok, better when KS

→ Consistency of the ingredients is most crucial

El Sahili, Sottile, Reining, J. Chem. Theory Comput. 20, 1972 (2024)

Combining many-body perturbation theory and TDDFT: getting the best of both worlds

→ Historical examples in modern perspective:

* fxc from the Bethe-Salpeter equation of MBPT

* vertex corrections beyond GW from TDDFT

→ Our today's research:

* fxc approx. vertex corrections: exotic excitations in the HEG

* How wrong are fxc approx. vertex corrections *in principle?*

→ A central quantity: $\Sigma[n]$

$$\frac{\delta\Sigma}{\delta G}\frac{\delta G}{\delta v} = \frac{\delta\Sigma}{\delta n}\frac{\delta n}{\delta v} = \left(v_c + \frac{\delta\Sigma_{\mathrm{xc}}}{\delta n}\right)\chi$$

In COHSEX or Hybrid fctls etc, central quantity is the 1-RDM

$$\rho[n] \longrightarrow \Sigma = \Sigma[n]$$

Machine learn $\rho[n]$

Wetherell, Costamagna, Gatti, Reining, Faraday Discussions 224, 265 (2020)

Or build approximate explicit density functionals

Elena Martini

Low density expansion of the non-interacting 1-RDM

Ayoub Aouina

HEG: $\rho(r, r') = n(r)$

Inhom., 1 electron approx.: $\rho^{\text{approx}}(\mathbf{r}_1, \mathbf{r}_2; [n]) = \sqrt{n(\mathbf{r}_1)n(\mathbf{r}_2)}$

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* vertex corr

Move between functionals!

→ We are not heading for the exact solution

But for a reasonably good and very fast one

→ Our today's r

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Combining many-body perturbation theory and TD DFT: getting the best of both worlds

Marc Aichner, Ayoub Aouina, Abdallah El Sahili, Matteo Gatti, Jaakko Koskelo, Elena Martini, Martin Panholzer, Claudia Roedl, Francesco Sottile, Marilena Tzavala, Lucia Reining

This kept us busy for 20 years

....and will continue!