Dynamical vertex corrections beyond GW from time-dependent density-functional theory

Georg S. Michelitsch, Lucia Reining and Matteo Gatti

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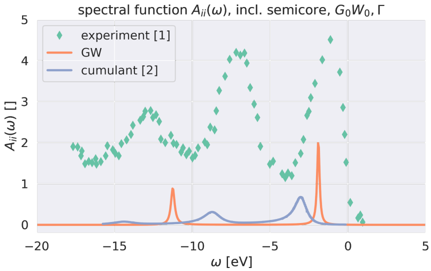
The problem with satellites ..

- Satellites in photoemission spectra are often (but not necessarily!) plasmon excitations
- Satellites are very sensitive to system details[2]
- GW has a satellite: → not the plasmon satellite!
- Plasmons were previously explained with the GW+C approach[3,4] → modification of G
- GW+C is limited to a coupling to plasmons
- Alternative: Use vertex corrections (avoid cumulant)

experimental photoemission spectrum of sodium[1]



Can we explain plasmon satellites by (dynamical) vertex corrections in W, instead of the GW+C approach?

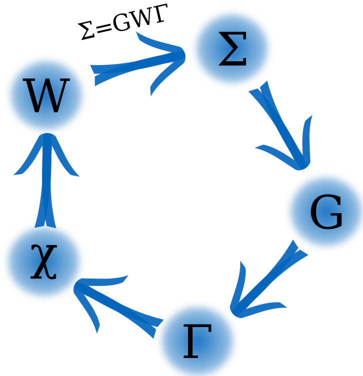
[1] Höchst H. et al. *Z. Phys.B: Condens. Matter* 30 (**1978**), 145
[2] Zhou J. et al. *Phys. Rev. B* 97(3) (**2018**), 035137
[3] Aryasetiawan F. et al. *Phys. Rev. Lett.* 77 (**1996**), 2268
[4] Guzzo M. et al. *Phys. Rev. Lett.* 107 (**2011**), 166401

Vertex corrections $\Sigma = GW\Gamma$ ... ?

- In the common GW-approximation[1]: $\Gamma = 1$
- Γ is needed to calculate Σ ("outer") and χ ("inner")
- In a qualitative picture:
  - The inner vertex describes the response of a the system as fermionic
  - The outer vertex describes the charge which feels the response as a fermion
- $\Gamma \rightarrow \frac{\delta\Sigma}{\delta G}$ Approximate as $\frac{\delta v_{xc}(r,t)}{\delta n(r',t')} = f_{xc}(r, r'; t - t')$
- Common in the past: Adiabatic LDA

$$f_{xc}^{ALDA} \propto \delta(r - r')\delta(t - t')$$

- Commonly in $GW\Gamma$ the f_{xc} is static[2–5], but f_{xc} should be ω dependent[6,9] and not completely local[7–9]



Can we include a q- and ω-dependent f_{xc} from TDDFT[7] in the GW calculation?

[1] Hedin L. *Phys. Rev.* 139 (**1965**), A796
[2] Hybertsen M. S. et al. *Phys. Rev. B* 34 (**1986**), 5390
[3] Del Sole R. et al. *Phys. Rev. B* 49 (**1994**), 8024
[4] Morris A. et al. *Phys. Rev. B* 76 (**2007**), 155106
[5] Maggio E. et al. *J. Chem. Theory Comput.* 13(10) (**2017**), 4765
[6] Maebashi H. et al. *Phys. Rev. B* 84 (**2011**), 245134
[7] Reining L. et al. *Phys. Rev. Lett* 88 (**2002**), 066404
[8] Schmidt P. et al. *Phys. Rev. B* 96 (**2017**), 205206
[9] Panholzer M. et al. *Phys. Rev. Lett.* 120 (**2018**), 166402

Effect of the inner vertex studied by a tabulated f_{xc}-kernel [1]

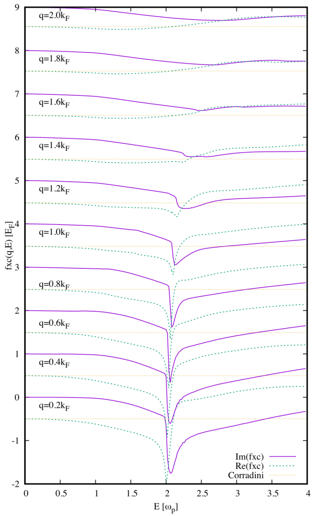
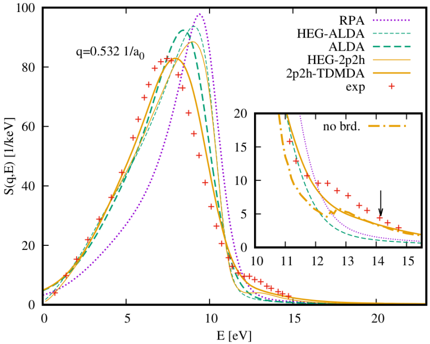


FIG. 1: The $2p2h$ kernel as a function of energy at $r_s = 4$ and at momenta starting from $q = 0.2k_F$ up to $q = 2k_F$ in steps of $\Delta q = 0.2k_F$ is shown. With increasing momentum the lines are offset in y-direction by $1E_F$.

Plasmon and double plasmon in IXS of Na $\propto$ Im[χ]



$\rightarrow$ correlated EOM with 1 & 2 particle excitations[2]

$\rightarrow$ TDDFT f_{xc} of the HEG (tabulated[3]): "2p2h-kernel"

$\rightarrow$ dominant feature of the kernel is a pole at $2\omega_p$

$\rightarrow$ Using this f_{xc}: plasmon and double-plasmon in S(q,ω)[2]

$\rightarrow$ f_{xc} must be ω-dependent to describe the double plasmon

[1] Panholzer M. et al., *Phys. Rev. Lett.* 120 (**2018**), 166402

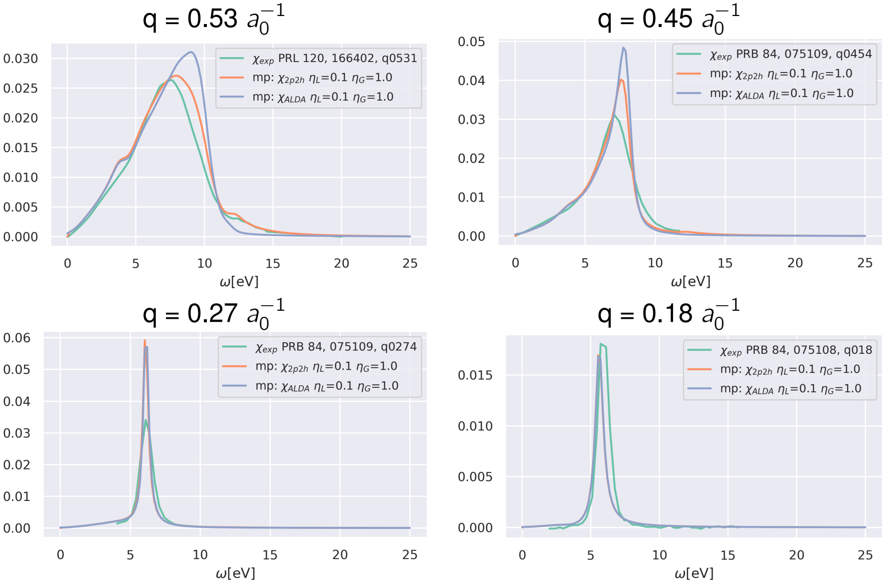
[2] Böhm H. M. et al. *Phys. Rev. B* 82, (**2010**), 224505

[3] https://etsf.polytechnique.fr/research/connector/2p2h-kernel

$\Rightarrow$ This f_{xc} kernel is both q- and ω-dependent!

Can we reproduce χ_{2p2h} with a multipole model?

$$\chi_{2p2h} = \frac{\chi_0}{1 - v\chi_0 - f_{xc}\chi_0}$$



- model reproduces χ_{2p2h} $\rightarrow$ systematically better than ALDA compared to experiment
- effect of f_{xc} in χ is weak for small values of q $\Rightarrow$ χ_0 is important!

In the small q, the f_{xc}-effect is small $\Rightarrow$ Maybe in the outer vertex this is different?

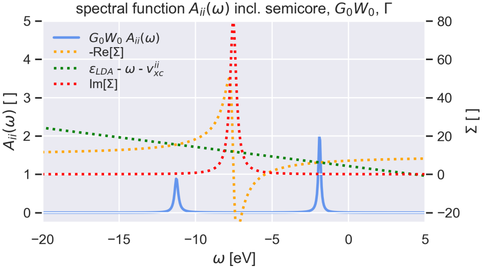
The outer vertex

- Add analytical term of the same structure as the 2p2h-kernel

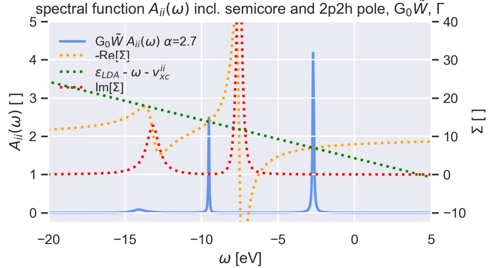
$$\tilde{W}(\omega') = [1 + (v + \alpha f_{xc}(\omega'))\chi(\omega')]v \qquad \Rightarrow \qquad \Sigma = GW\Gamma = G\tilde{W}$$

α is not a free parameter $\rightarrow$ determined from $f_{xc}(\omega = 0)$

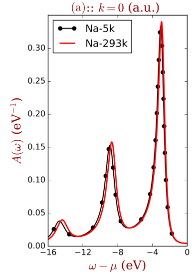
without kernel



including kernel



cumulant[1]



$\rightarrow$ satellite peak $\neq \omega_p$ ($\simeq$ 6eV)

$\rightarrow$ no 2 * ω_p satellite

$\rightarrow$ satellite shifted towards ω_p

$\rightarrow$ quasiparticle distance decreased

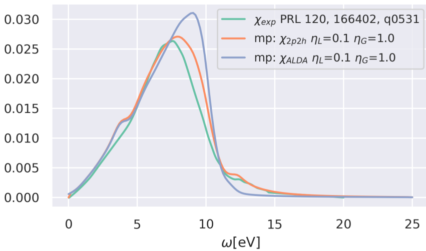
$\rightarrow$ 2 * ω_p satellite appears

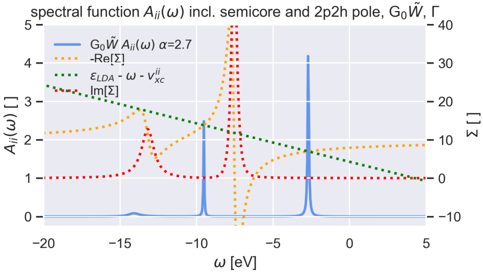
All seen effects are caused purely because of the ω-dependence of f_{xc}!

[1] Zhou J. et al. *Phys. Rev. B* 97(3) (**2018**), 035137

Conclusion

- $\rightarrow$ The inner model vertex introduces $2\omega_p$ in $\tilde{\chi}$
  - $\rightarrow$ The effect of the inner vertex is small for small q
- $\rightarrow$ The outer model vertex predicts qualitatively correct spectral function
  - $\rightarrow$ The outer vertex shifts the plasmon satellite and creates the $2\omega_p$
- $\rightarrow$ Vertex corrections with $f_{xc}(\omega)$ are a different way to get the same result as the cumulant but open a possible route towards coupling to other bosons
- $\rightarrow$ Other materials are not so close to the HEG
  - $\rightarrow$ if needed, a connector can be employed[1−4]





[1] Ayoub Aouina, *MSc Thesis* (**2019**), Development of functionals for observables

[2] Marco Vanzini, *PhD Thesis* (**2018**), Auxiliary systems for observables: dynamical local connector approximation for electron addition and removal spectra

[3] Panholzer M. et al., *Phys. Rev. Lett.* 120 (**2018**), 166402

[4] Vanzini M. et al., *arXiv:cond-mat.other* (**2019**), 1903.07930

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Thank you for your attention!