Using a tabulated f_{xc} to calculate ϵ^{-1}

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Using ϵ^{-1} to connect theories

Coming from TDDFT: $\tilde{\chi} = \chi_0 + \chi_0[v + f_{xc}]\tilde{\chi}$
with $f_{xc}(q, \omega)$ from the tabulated data [1,2]

$f_{xc}(q, \omega, r_s) \Rightarrow$ HEG-kernel for the mean density of the real system.

[1] Panholzer M. et al., *Phys. Rev. Lett.* 120 (**2018**), 166402
[2] https://etsf.polytechnique.fr/research/connector/2p2h-kernel

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"testparticle" ϵ^{-1} [1]

$$\epsilon^{-1}_{TC}(q,\omega) = 1 + v(q)\tilde{\chi}(q,\omega)$$

- dynamic structure factor (DSF)
- corrected ω_p
- introduced (small) $2\omega_p$

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"testelectron" ϵ^{-1}

$$\epsilon^{-1}_{TE}(q,\omega) = 1 + [v(q) + f_{xc}(q,\omega)]\tilde{\chi}(q,\omega)$$

- go beyond GW: $\tilde{W} = \epsilon^{-1}_{TE}v = [1 + [v + f_{xc}]]\tilde{\chi}v$
- photoemission spectra with G$\tilde{W}$
- corrected plasmon satellite?
- second satellite?

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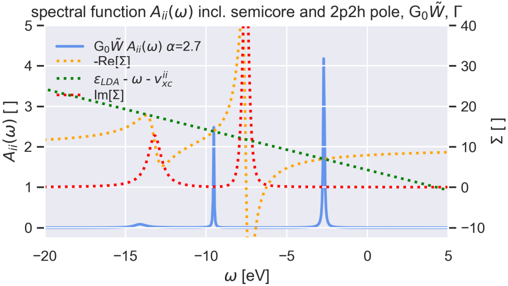
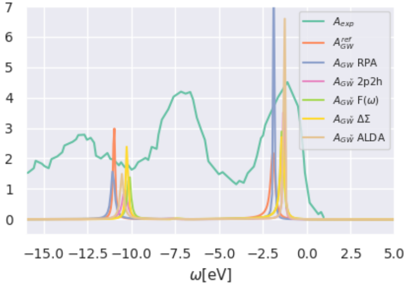
Results of a model study

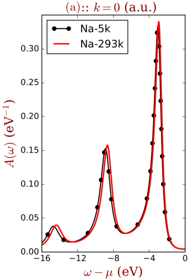
analytic model



parametrized model



cumulant[1]



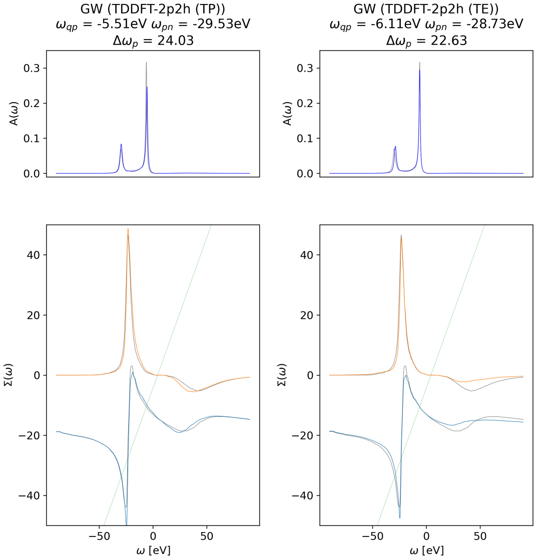
- Analytic model demonstrated general feasability
- Parametrized model suggests the effect of the actual f_{xc} will be weak
- Cumulant expansion is the state-of-the-art[1]

$\Rightarrow$ Implementation of ϵ^{-1}_{TE} with 2p2h-f_{xc} in dp-code

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

Results of the ab-initio implementation

Si, G0W0

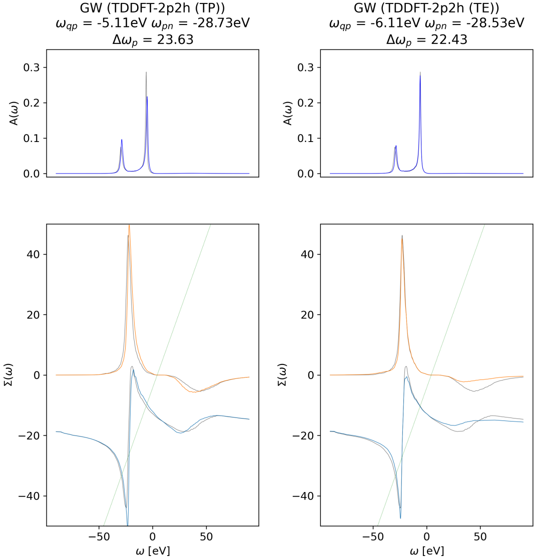


- small changes to spectral function
- inner and outer vertex (ϵ^{-1}_{TP} vs. ϵ^{-1}_{TE}) compensate (!)
- sharper or stronger f_{xc} features required?
- $\bar{\rho}$ good connector? $\Rightarrow$ Na very HEG-like

What has gone wrong?

Results of the ab-initio implementation

Si, evGW0



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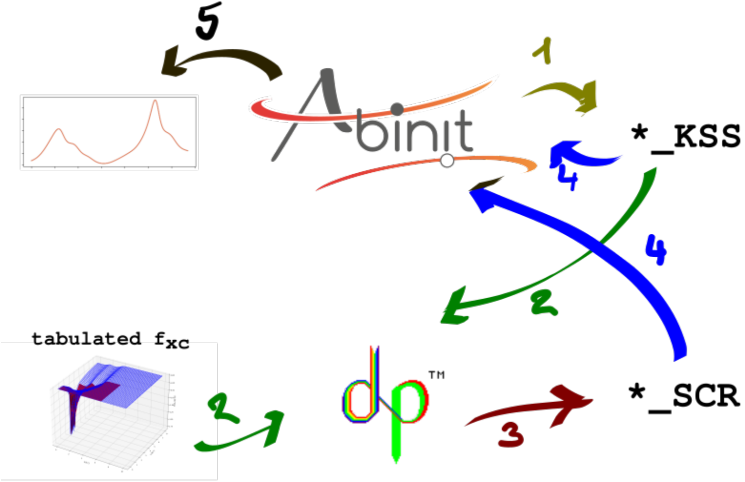
Thank you for your attention!

Parkplatz für Slides ohne Plätzchen

Flowchart of workflow



A fully parametrized GW-model including vertex corrections

1| response function χ

χ_0 for Na $\rightarrow$ multipole-model

$\chi_{RPA} = \chi_0/(1 - v_i\chi_0)$

2| exchange-correlation kernel

f_{xc} for HEG[1,2] $\rightarrow$ multipole-model

3| the inner vertex

$\chi_{2p2h} = \chi_0/(1 - v_i\chi_0 - \beta f_{xc})$

IXS and ab-initio data for Na[1,3]

4| the outer vertex

$\Sigma^c_{GW\Gamma^{in}_{out}} / \Sigma^c_{GW\Gamma^{in}} \simeq 1 - \alpha\,/\,(2v\omega_p)$

$\Sigma_{GW\Gamma}$ calculated with ALDA[4]

5| self-energy

$W = v(1 + v_o)\chi_{RPA}$

$\tilde{W} = v(1 + v_o + \alpha f_{xc})\chi_{2p2h}$

$\Sigma = \int G(\omega')\tilde{W}(\omega - \omega')d\omega'$

6| spectral function $A(\omega)$

$A(\omega) = f(\omega, v_i, v_o, \alpha, \beta, f_{xc}, \chi_0)$

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

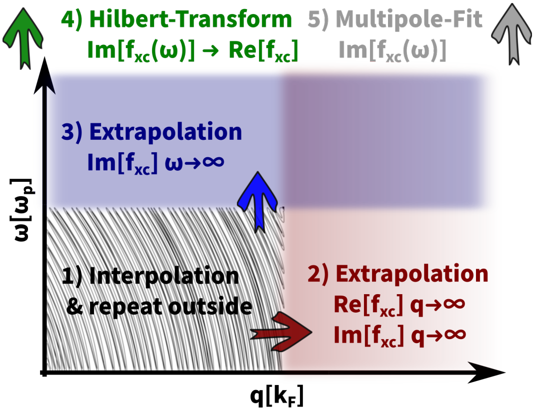
[2] https://etsf.polytechnique.fr/research/connector/2p2h-kernel

[3] Cazzaniga M. et al., *Phys. Rev. B* 84 (**2011**), 075109

[4] Del Sole R. et al., *Phys. Rev. B* 49 (**1994**), 8024

parameters (4), published data (2), ab-initio data (2)

Tabulated kernel usage - final approach

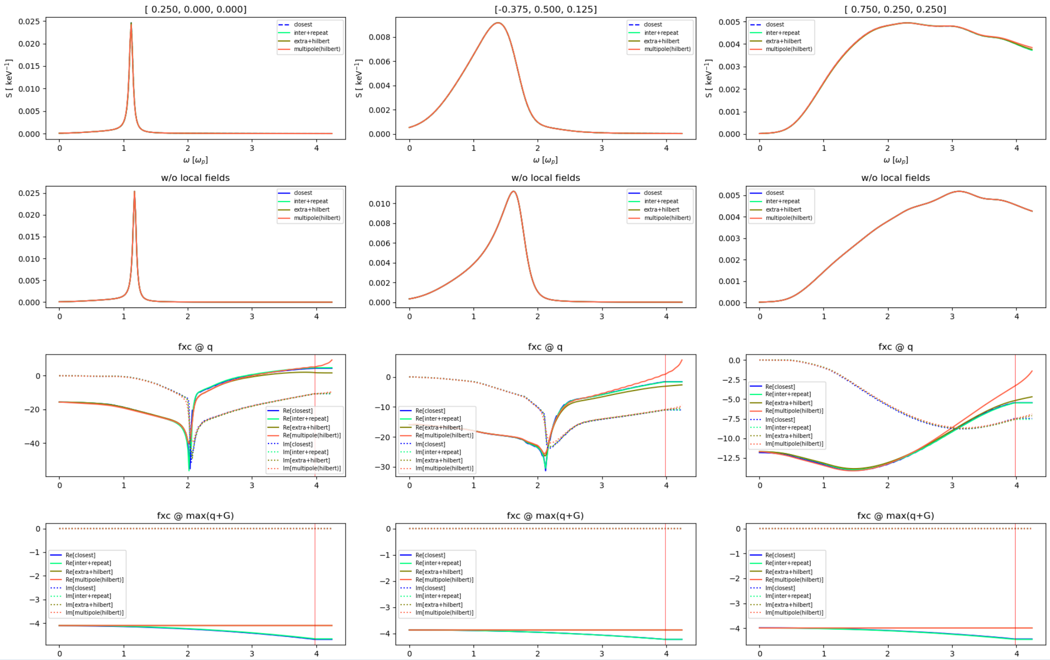


- Most "physical" version:
  4) Hilbert-Transform
  - calculation of spectra in dp
- Required for GW:
  5) Multipole-Fit & AC
  - calculation of outer vertex in ϵ^{-1}
- Pitfalls: 2) and 3)
  - look at limits in both Re/Im parts

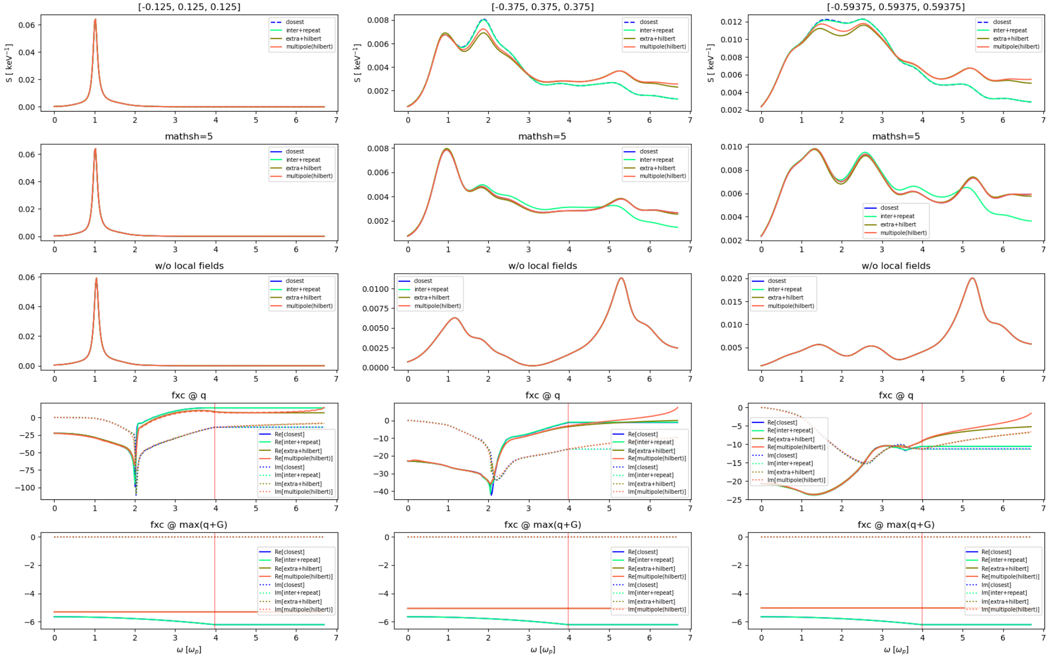
Comparison of different approaches

- `closest`
  closest tabulated values are chosen
- `inter+repeat`
  interpolation of values inside table, repetition outside
- `extra+hilbert`
  interpolation of values inside table, extrapolation of Im outside + Hilbert transform to Re
- `multipole(hilbert)`
  multipole-expansion of the Im-part from extra+hilbert

Example: DSF of Na and K at different q-points



[0.250, 0.000, 0.000]
[-0.375, 0.500, 0.125]
[0.750, 0.250, 0.250]
S [keV^{-1}]
ω [ω_p]
closest
inter+repeat
extra+hilbert
multipole(hilbert)
w/o local fields
fxc @ q
fxc @ max(q+G)
Re[closest]
Re[inter+repeat]
Re[extra+hilbert]
Re[multipole(hilbert)]
Im[closest]
Im[inter+repeat]
Im[extra+hilbert]
Im[multipole(hilbert)]


[-0.125, 0.125, 0.125]
[-0.375, 0.375, 0.375]
[-0.59375, 0.59375, 0.59375]
mathsh=5
w/o local fields
fxc @ q
fxc @ max(q+G)
S [keV^{-1}]
closest
inter+repeat
extra+hilbert
multipole(hilbert)
Re[closest]
Re[inter+repeat]
Re[extra+hilbert]
Re[multipole(hilbert)]
Im[closest]
Im[inter+repeat]
Im[extra+hilbert]
Im[multipole(hilbert)]
ω [ω_p]

Analytic continuation of f_{xc}

A single anti-resonant pole function ϕ_1 along the real axis :

$$\phi_1(\omega,\eta,\omega_p) = \frac{1}{\omega-\omega_p+i\eta} - \frac{1}{\omega+\omega_p-i\eta} = \frac{2\omega_p - 2i\eta}{\omega^2-(\omega_p-i\eta)^2} \tag{1}$$

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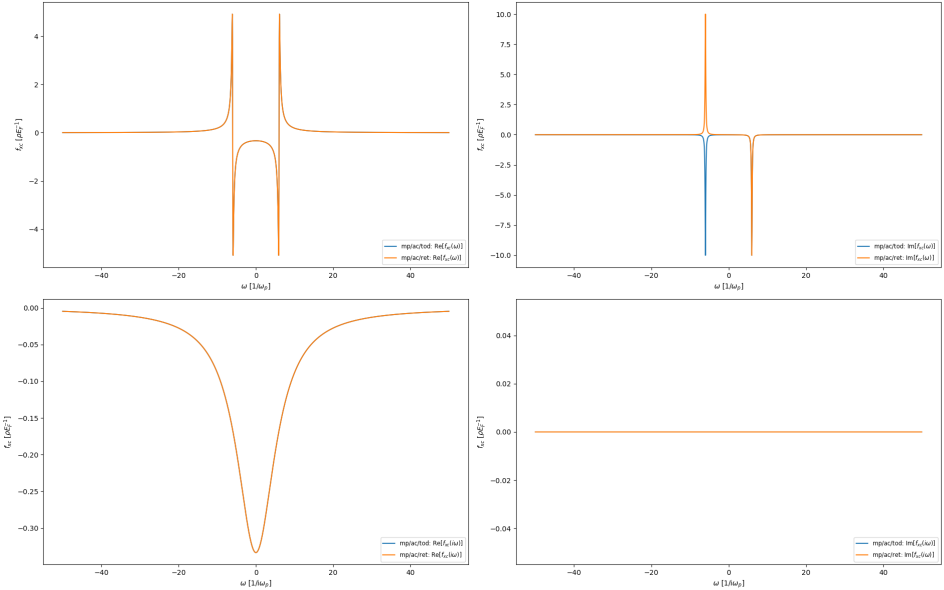
The function is defined for a variable $z = \omega + i\eta\text{sgn}(\omega)$ and parameter ω_p. Writing down $\phi_1(z, \omega_p)$, the *analytic continuation* becomes apparent:

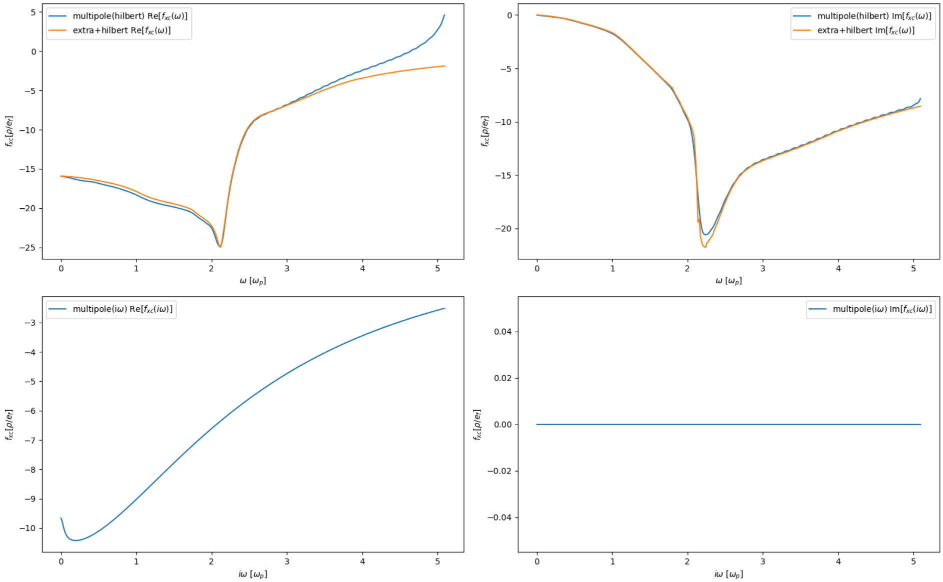
$$\text{along real axis } (\eta \neq 0): \quad \phi_1(z, \omega_p) = \frac{1}{\omega + i\eta\,\text{sgn}(\omega) - \omega_p} - \frac{1}{\omega + i\eta\,\text{sgn}(\omega) + \omega_p} = \frac{1}{z - \omega_p} - \frac{1}{z + \omega_p} = \frac{2\omega_p}{z^2 - \omega_p^2} \tag{2}$$

$$\text{on imag. axis } (z = 0 + i\omega): \quad \phi_1(0 + i\omega, \omega_p) = \frac{2\omega_p}{(i\omega)^2 - \omega_p^2} = \boxed{\frac{2\omega_p}{\omega^2 - \omega_p^2}} \tag{3}$$

Single anti-resonant pole



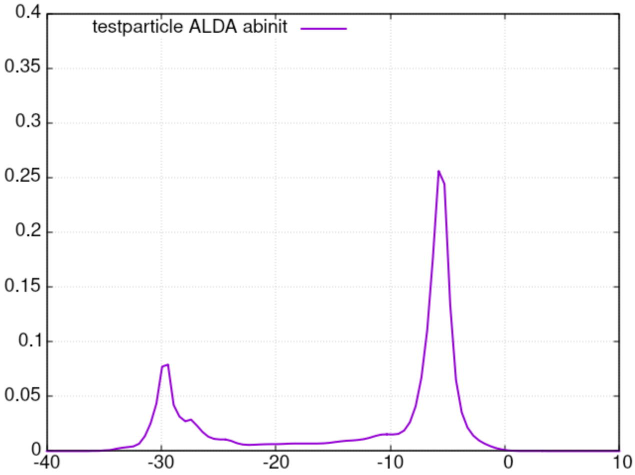
f_{xc} at $r_s = 4.0$



multipole(hilbert) Re[$f_{xc}(\omega)$]
extra+hilbert Re[$f_{xc}(\omega)$]
multipole(hilbert) Im[$f_{xc}(\omega)$]
extra+hilbert Im[$f_{xc}(\omega)$]
multipole($i\omega$) Re[$f_{xc}(i\omega)$]
multipole($i\omega$) Im[$f_{xc}(i\omega)$]
$f_{xc}[\rho/e_f]$
ω [ω_p]
$i\omega$ [ω_p]

ϵ^{-1} with outer vertex for GW

Testsystem: GWΓ Silicon tutorial from abinit, ALDA, 2p2h, spectral function



CAVE:

- unvalidated (2p2h) implementation
- underconverged settings

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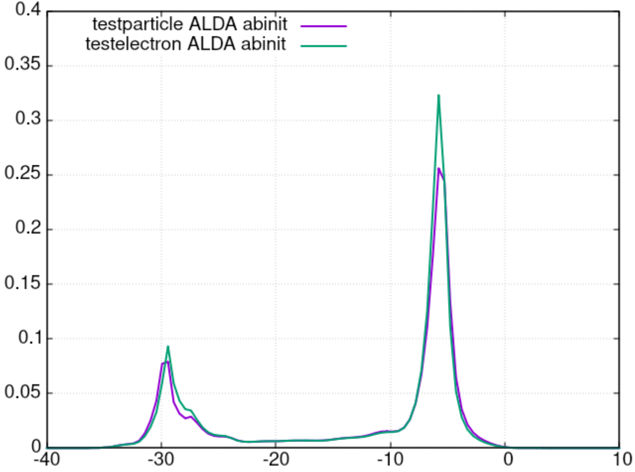

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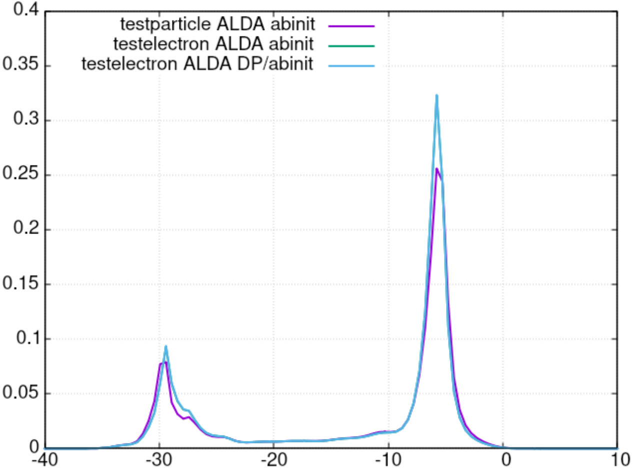

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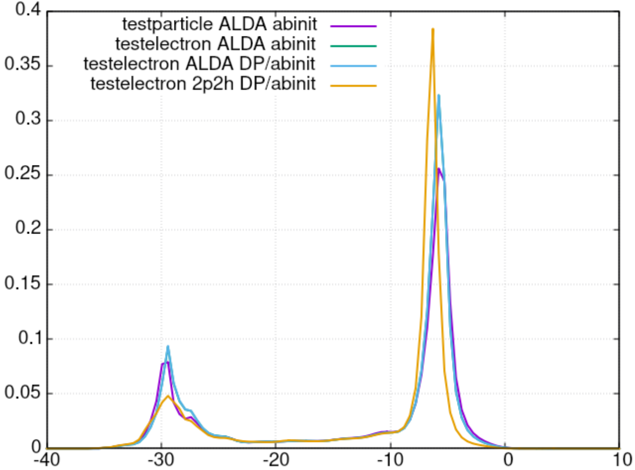

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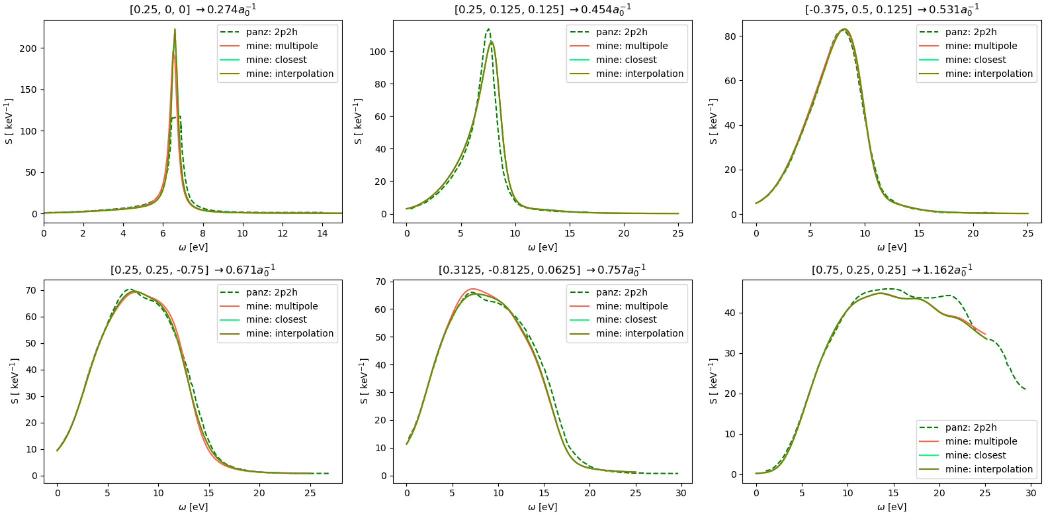
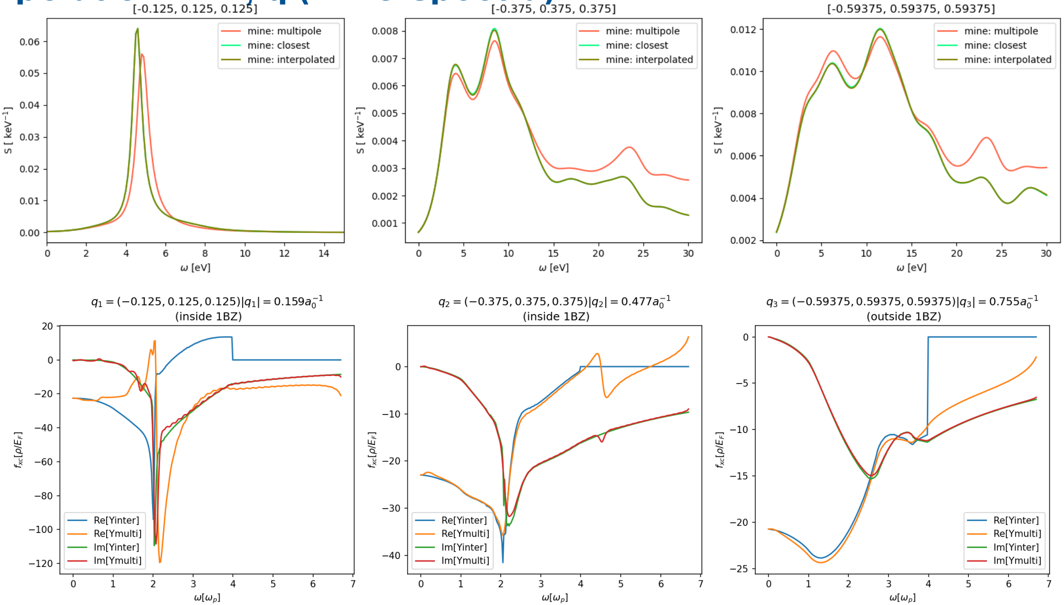
Conclusions

- Interpolation+Extrapolation+Hilbert-Transform for spectra
- Multipole-expansion of Im[f_{xc}] is stable
- Analytic continuation on $i\omega$ implemented
- testelectron screening file implemented & validated for ALDA
- Write screening file with 2p2h
- TODO: Validate implementation of `2p2h_SCR`

Interpolation in ω, q (Na TC spectra)



Interpolation in ω, q (K TC spectra)



"Multipole" expansion

$$\text{Im}[f_{xc}](\omega) \quad | \quad \omega \in \mathbb{C} \setminus \{\mp\omega_i \pm i\eta\} =$$

1. $\sum_i \frac{\alpha_i[4\omega_i - 4i\eta]}{\omega^2 - (2\omega_i - i\eta)^2}$

- needs many poles for $\lim_{\omega \to \pm\infty}$

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Current prodecure: (adv: analytic continuation ?)

1. Fitting $\mathrm{Im}[f_{xc}](\mathrm{Re}[\omega])$ to tabulated $\mathrm{Im}[f_{xc}]$ using equations above
2. Evaluating (analytically) $\mathrm{Re}[f_{xc}](\mathrm{Re}[\omega])$

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Alternative procedure: (adv: faster, less poles)

1. Represent $\text{Im}[f_{xc}]$ piece-wise on tight & large auxiliary ω-grid
2. Use $\text{Re}[f_{xc}] = -\frac{1}{\pi}\int_{-\infty}^{+\infty} \frac{\text{Im}[f_{xc}(\omega')]}{\omega' - \omega} d\omega'$ via numerical convolution

"Analytic continuation" to Im[ω]

$$\sum_i \frac{\alpha_i[4\omega_i - 4i\eta]}{\omega^2 - (2\omega_i - i\eta)^2} \quad \begin{array}{l} \hat{\mathbb{D}} = \mathbb{C} \setminus \{\mp\omega_i \pm i\eta\} \\ \{\omega_i, \eta, \alpha\} \in \mathbb{R} \end{array}$$

- I only have data along the real axis $\mathbb{D} = \mathbb{R}$, $\mathbb{Z} = \mathbb{C}$
- The above equation holds also on $\hat{\mathbb{D}} = \mathbb{C} \setminus \{\mp\omega_i \pm i\eta\}$
- In the limit of ω being real, the equation gives the original data
- The imaginary axis (Im[ω]) is part of $\hat{\mathbb{D}}$
- Only possible for pure multipole-representation, not a piecewise function