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Statistical inference of collision frequencies from X-ray Thomson scattering spectra

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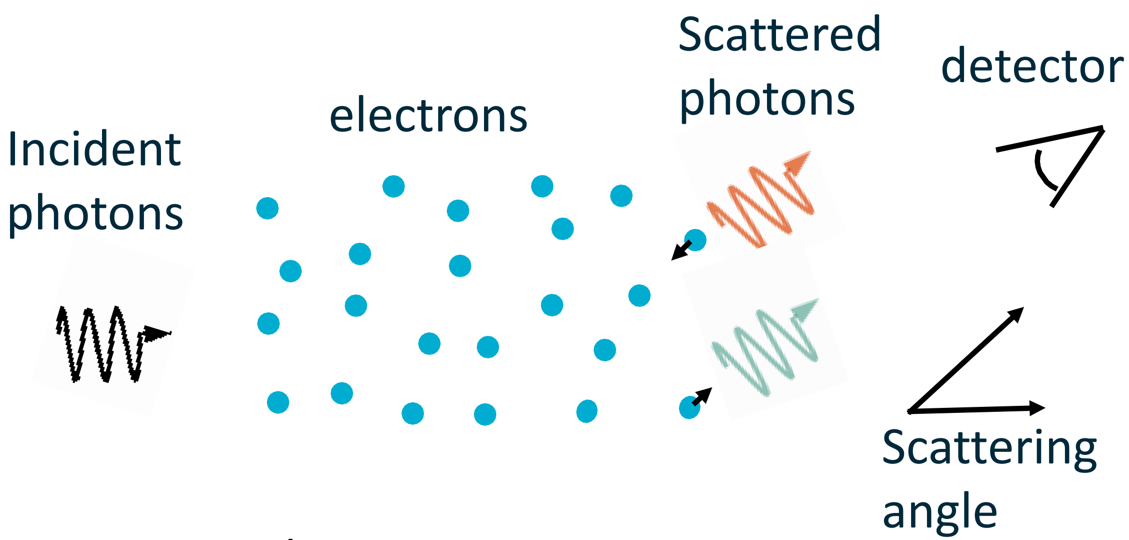
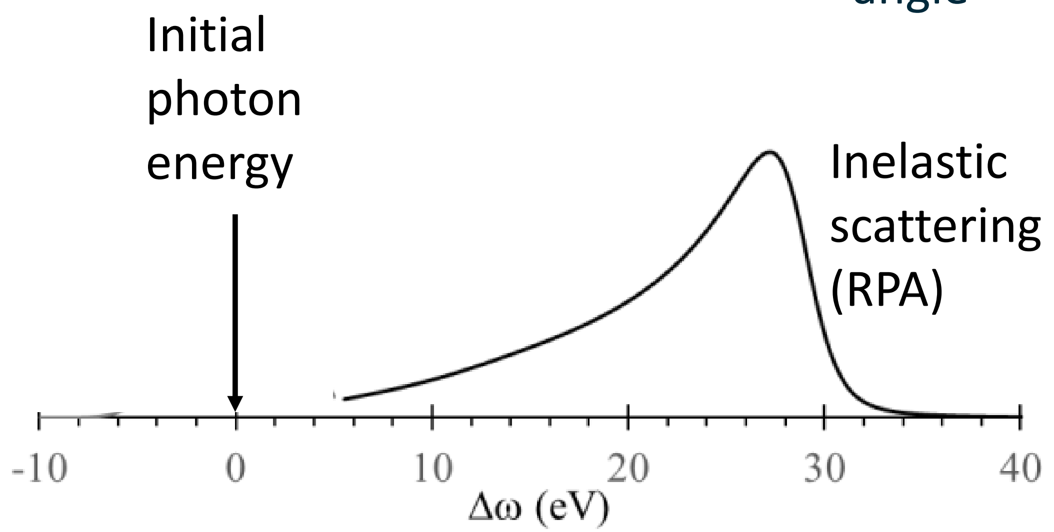
X-ray Thomson scattering (XRTS) is a useful diagnostic for dense plasmas

- X-rays scattering from free electrons are shifted by collective, Compton and Doppler effects, reflecting the electron energy distribution (Te & ne)

- In a uniform electron gas, scattering is accurately described by the random phase approximation (RPA)

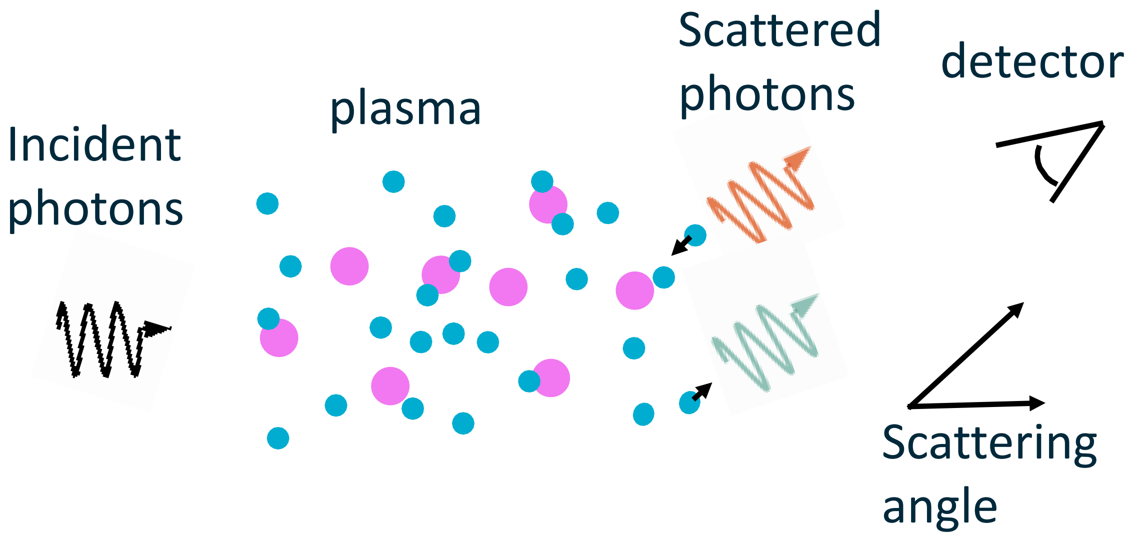


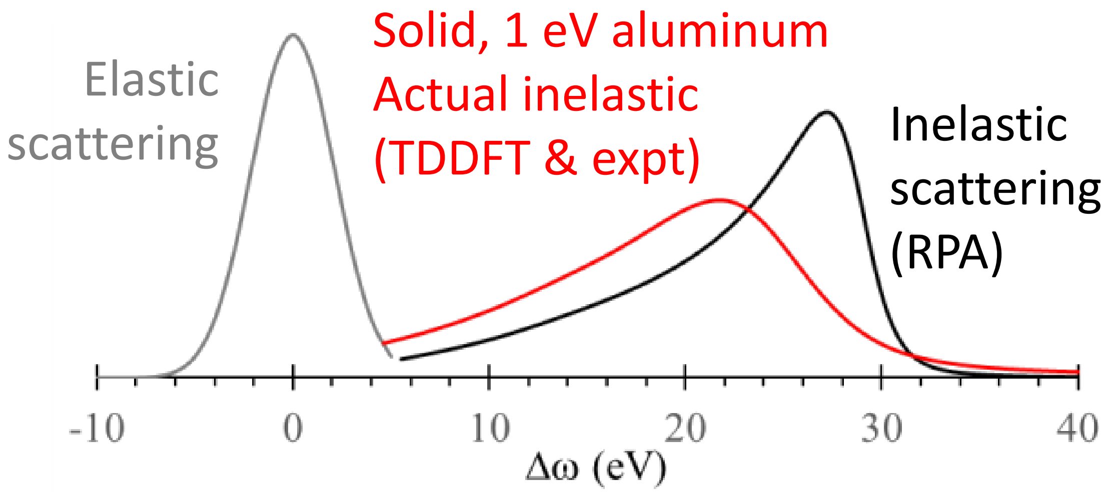


Glenzer & Redmer, Review of Modern Physics, 2009

X-ray Thomson scattering (XRTS) is a useful diagnostic for dense plasmas

- X-rays scattering from free electrons are shifted by collective, Compton and Doppler effects, reflecting the electron energy distribution (Te & ne)
- In a uniform electron gas, scattering is accurately described by the random phase approximation (RPA)
- Introducing ions adds complexity:
  - partial ionization
  - non-ideal densities of states
  - **electron-ion collisions (Mermin approx.)**



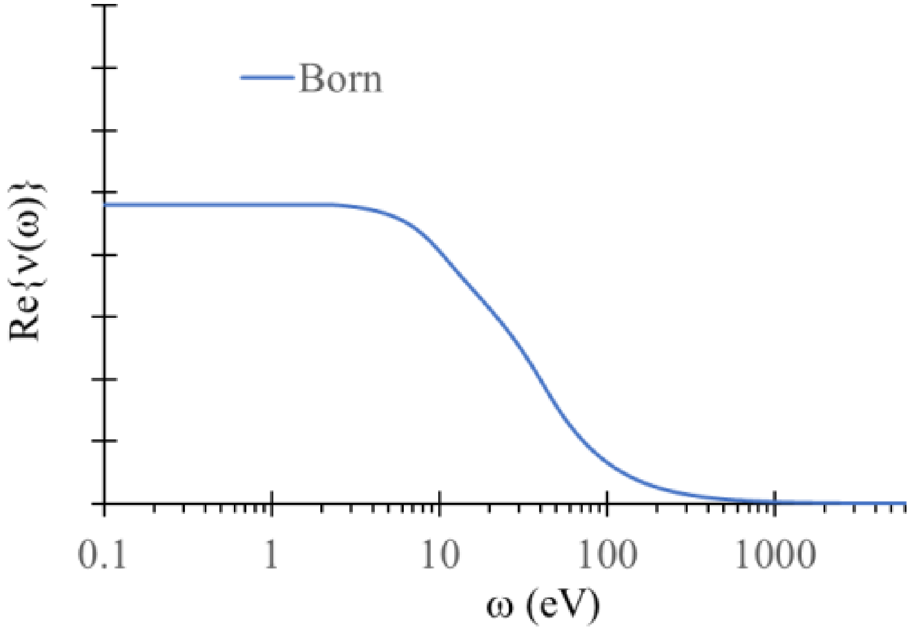


This talk explores how reliably XRTS spectra can constrain electron-ion collisions

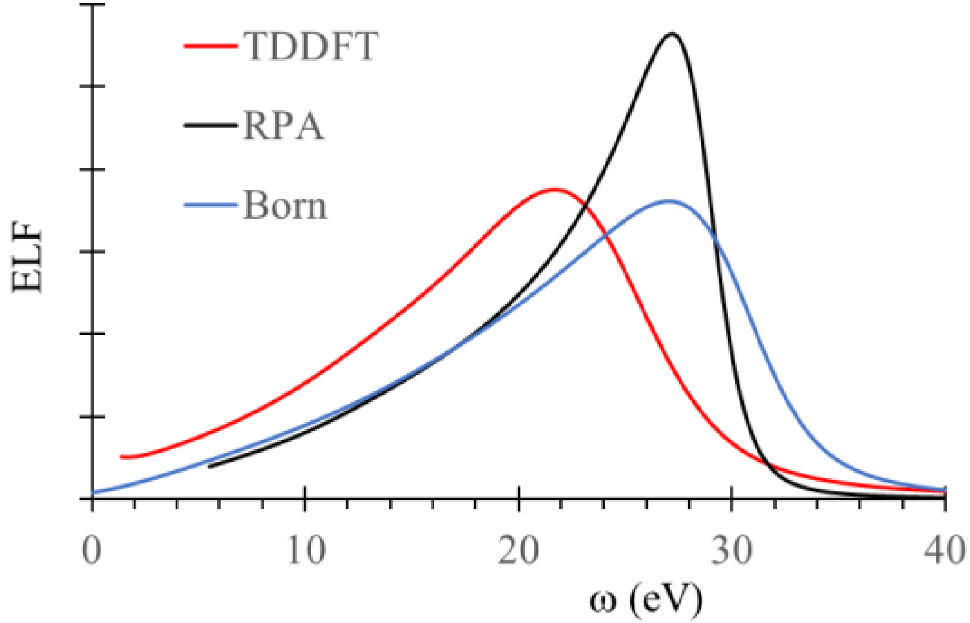
The Mermin equation translates a given dynamic collision frequency to a scattering signal

$$\epsilon^{M}(k,\omega) = 1 + \frac{(\omega + i\nu)\left[\epsilon^{0}(k,\omega+i\nu) - 1\right]}{\omega + i\nu \dfrac{\epsilon^{0}(k,\omega+i\nu) - 1}{\epsilon^{0}(k,0) - 1}},$$

RPA



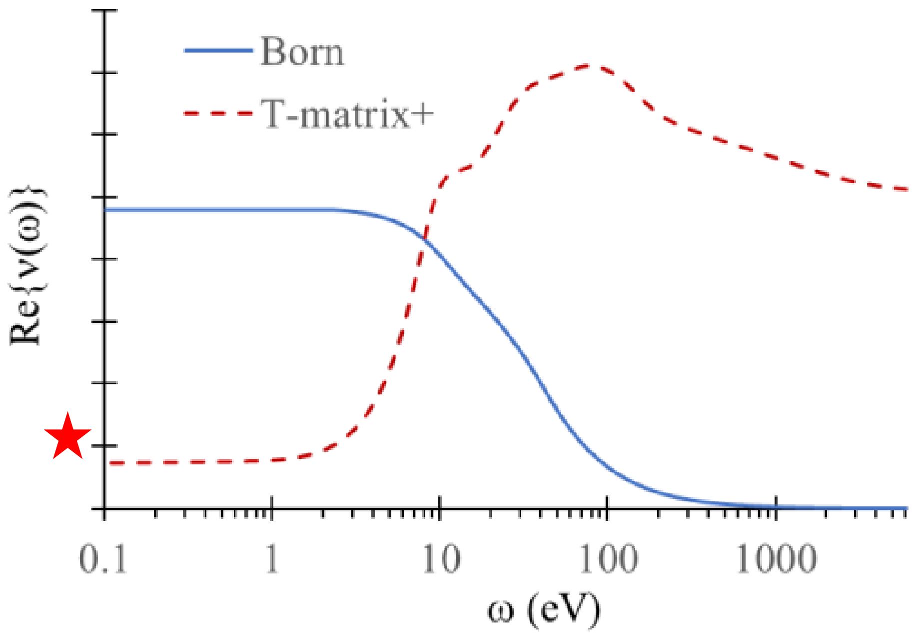
Given a forward calculation of ν(ω)...

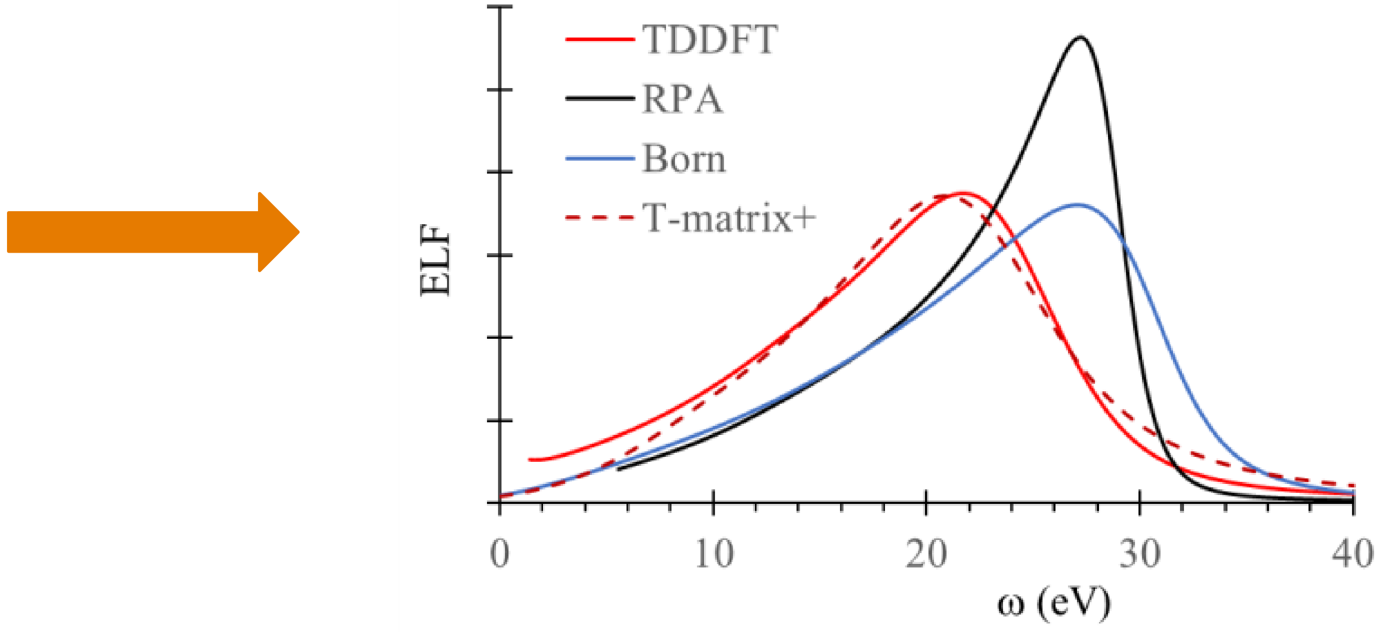


...we obtain an electron loss function (ELF), which is closely related to XRTS

Better models of the collision frequency can improve the agreement of the Mermin ELF with TDDFT

$$\epsilon^{\mathrm{M}}(k,\omega) = 1 + \frac{(\omega + i\nu)\left[\epsilon^{0}(k,\omega + i\nu) - 1\right]}{\omega + i\nu \dfrac{\epsilon^{0}(k,\omega + i\nu) - 1}{\epsilon^{0}(k,0) - 1}},$$

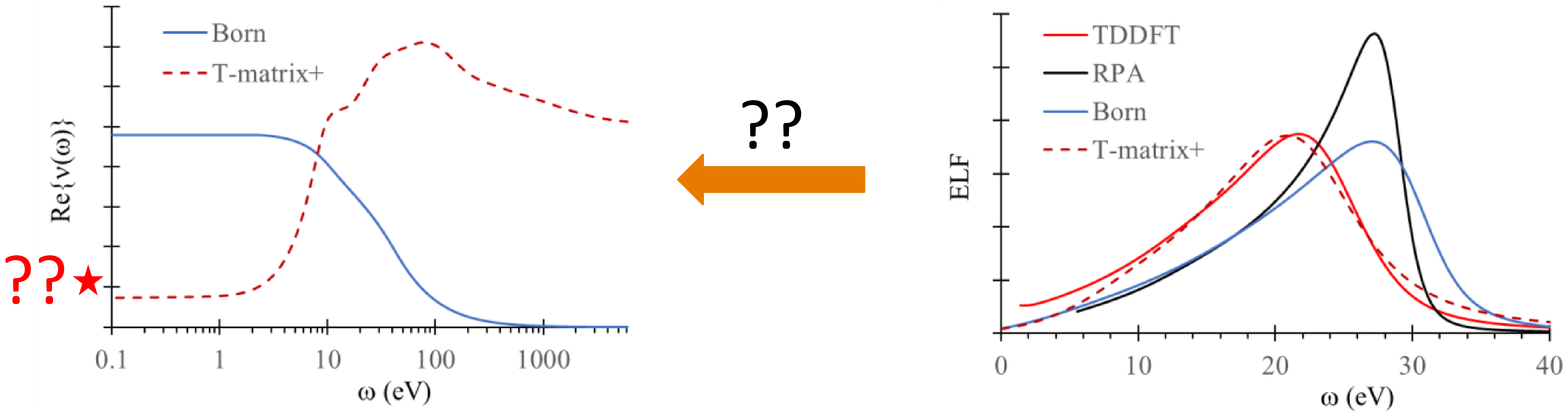




Better models for $\nu(\omega)$ include more detailed physics (cross sections, densities of state, partial ionization, ion structure factors…) and match other reference data, like the DC conductivity ★

Hentschel et al PoP 30, 062703 (2023)

Can we use scattering spectra to infer $\nu(\omega)$ and/or DC conductivities?



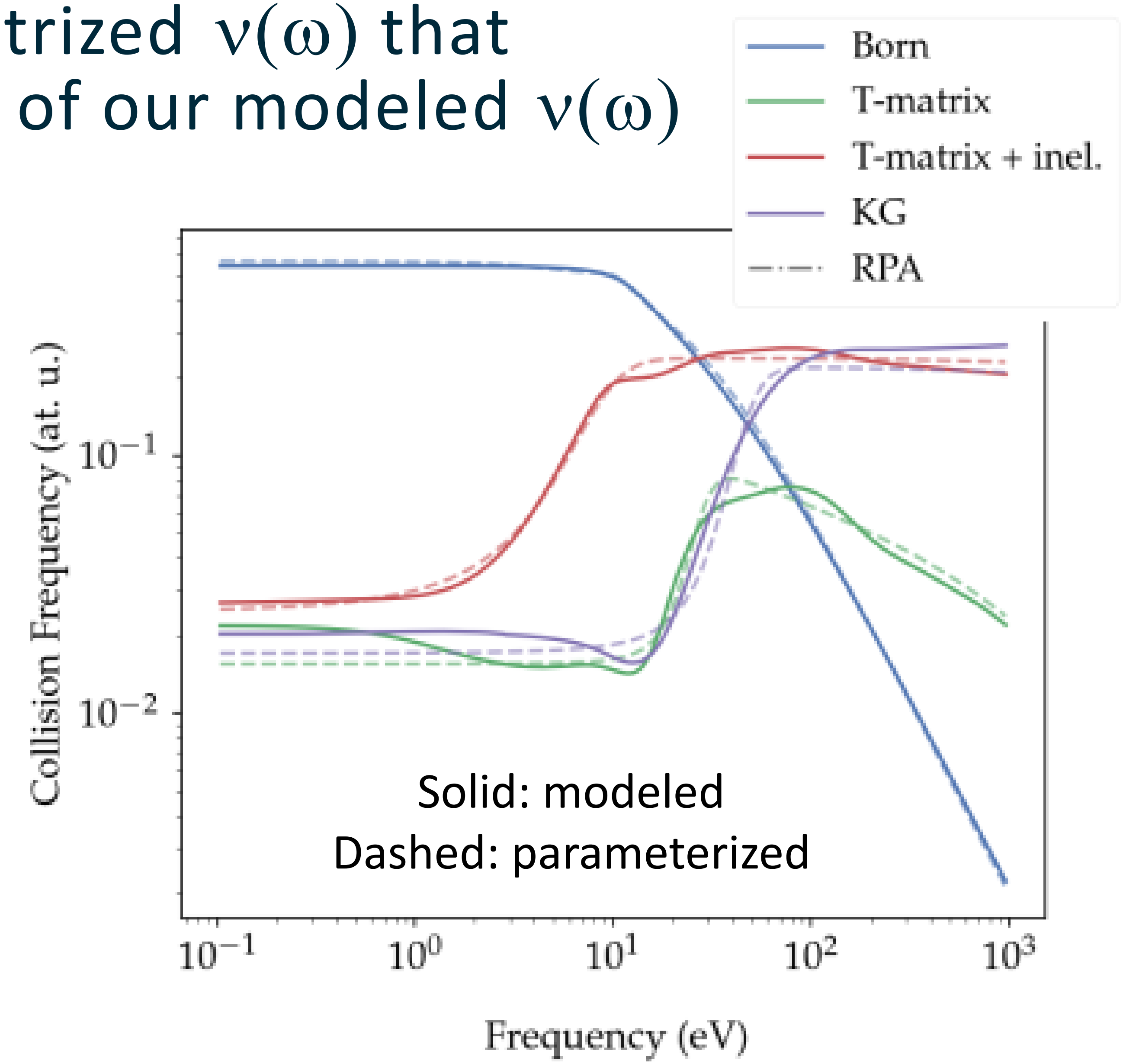
We define a flexible parametrized ν(ω) that captures the major features of our modeled ν(ω)

$$\nu(\omega) = \frac{\nu_0}{1 + \left(\frac{\omega}{b_0}\right)^{3/2}} + \frac{\nu_1}{1 + e^{-(\omega - \omega_\alpha)/\alpha} + \left(\frac{\omega}{\omega_\alpha}\right)^{p}}$$

"Born" term

"Activated" term

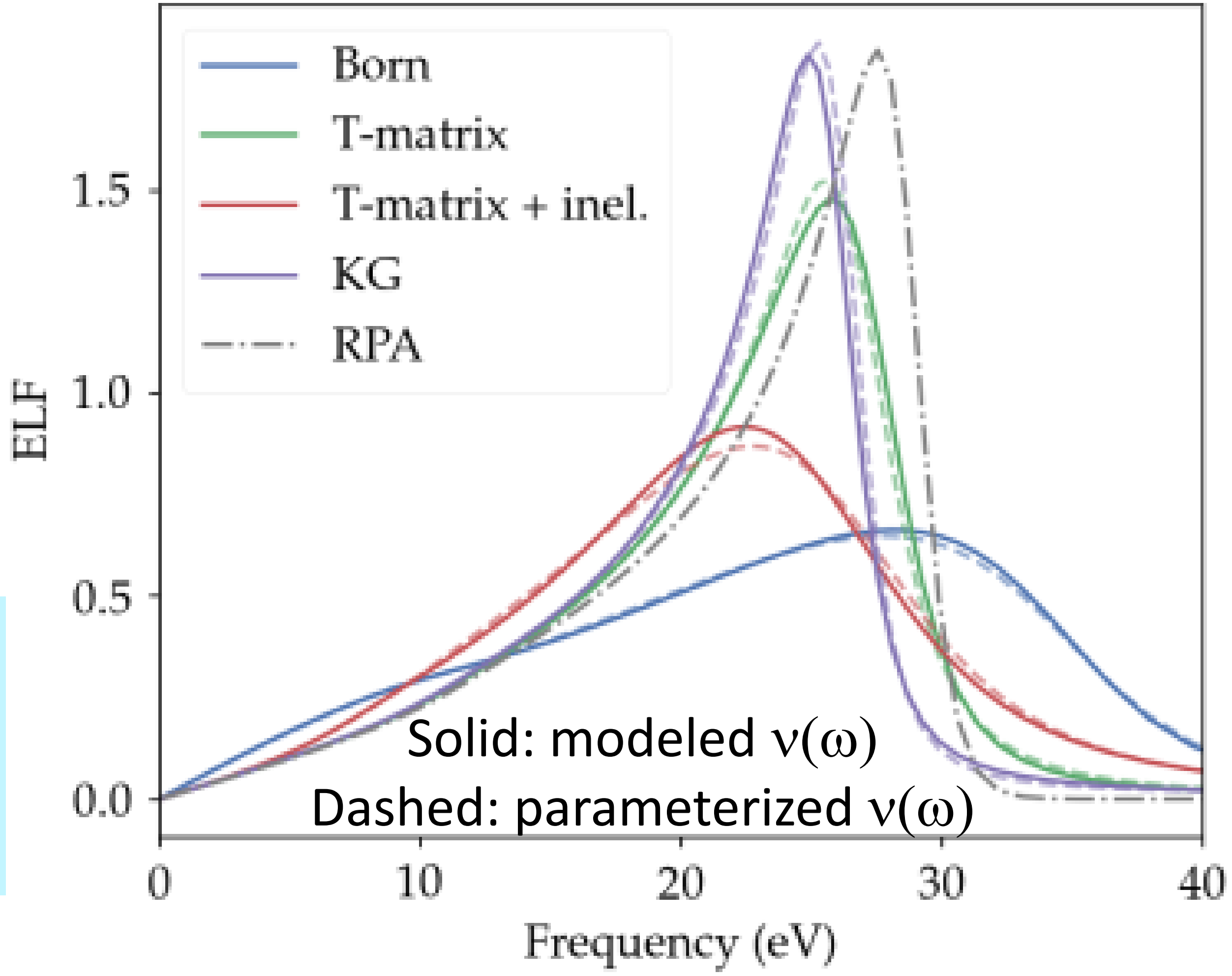
Note: b_0 is constrained by a sum rule



We verify that the parameterized ν(ω) can reproduce the Mermin scattering spectra with modeled ν(ω)

Applying Kramers-Kronig to the best-fit parameterized Re{ν(ω)}, we obtain Im{ν(ω)}, then use the Mermin approximation to check that the paramterized ν(ω) give reasonable scattering spectra.

The parameterized ν(ω) enables us to use Markov-Chain Monte Carlo and Bayesian methods to infer families of ν(ω), given a scattering spectrum

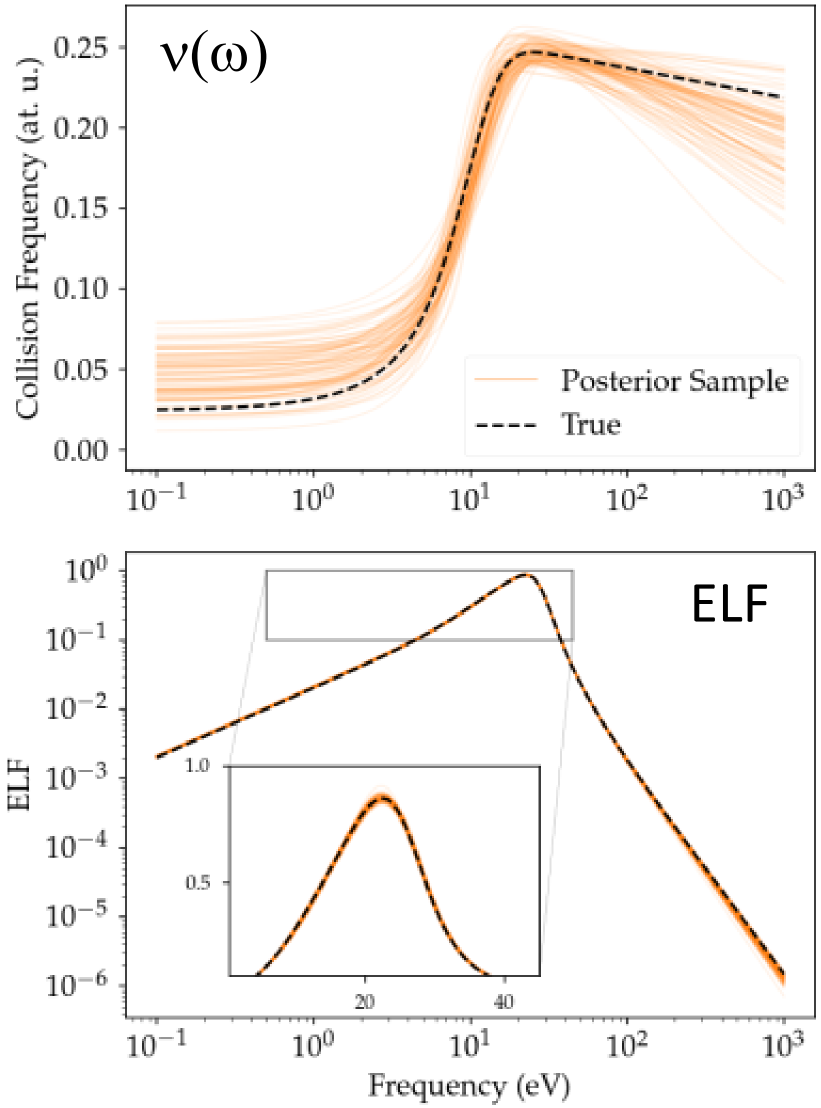


We test Markov-chain Monte Carlo sampling and Bayesian inference methods with an "ideal" case

The ELF for this ideal case is generated by one of our parameterized $\nu(\omega)$, so we know that it can be reproduced exactly

We use a relative residual to fit the ELF, so every part of the ELF has equal weight in the inference of $\nu(\omega)$

Even in this idealized case, we found significant variance in the inferred $\nu(\omega)$, especially at low and high frequencies



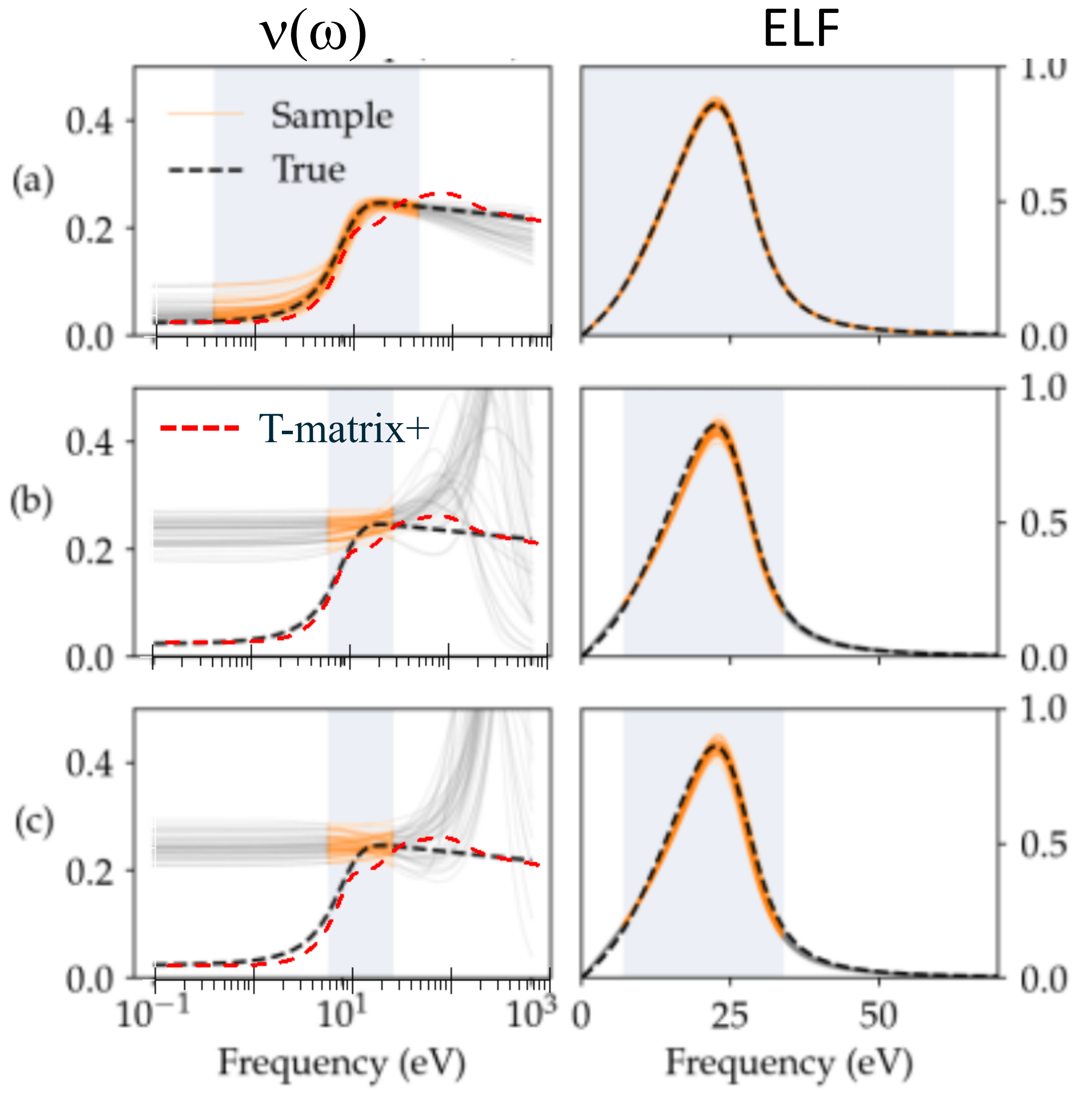
Since real scattering data is limited in range and often noisy, we explored modifications of the inference framework

Keeping the previous ELF as the objective, we restricted the frequency range used in the fitting:

a) To 99% of the peak ELF
b) To 80% of the peak ELF
c) To 80% of peak, using an absolute residual that implicitly weights larger ELF values

While each of these modifications can reproduce the ELF and find values near the "true" $\nu(\omega)$ in the fitted range, all have significant variance outside that range

The 80%-restricted cases do not find the "true" $\nu(\omega)$ in the low-frequency (DC) limit



Finally, we applied the restricted-inference method to data generated by a first-principles model

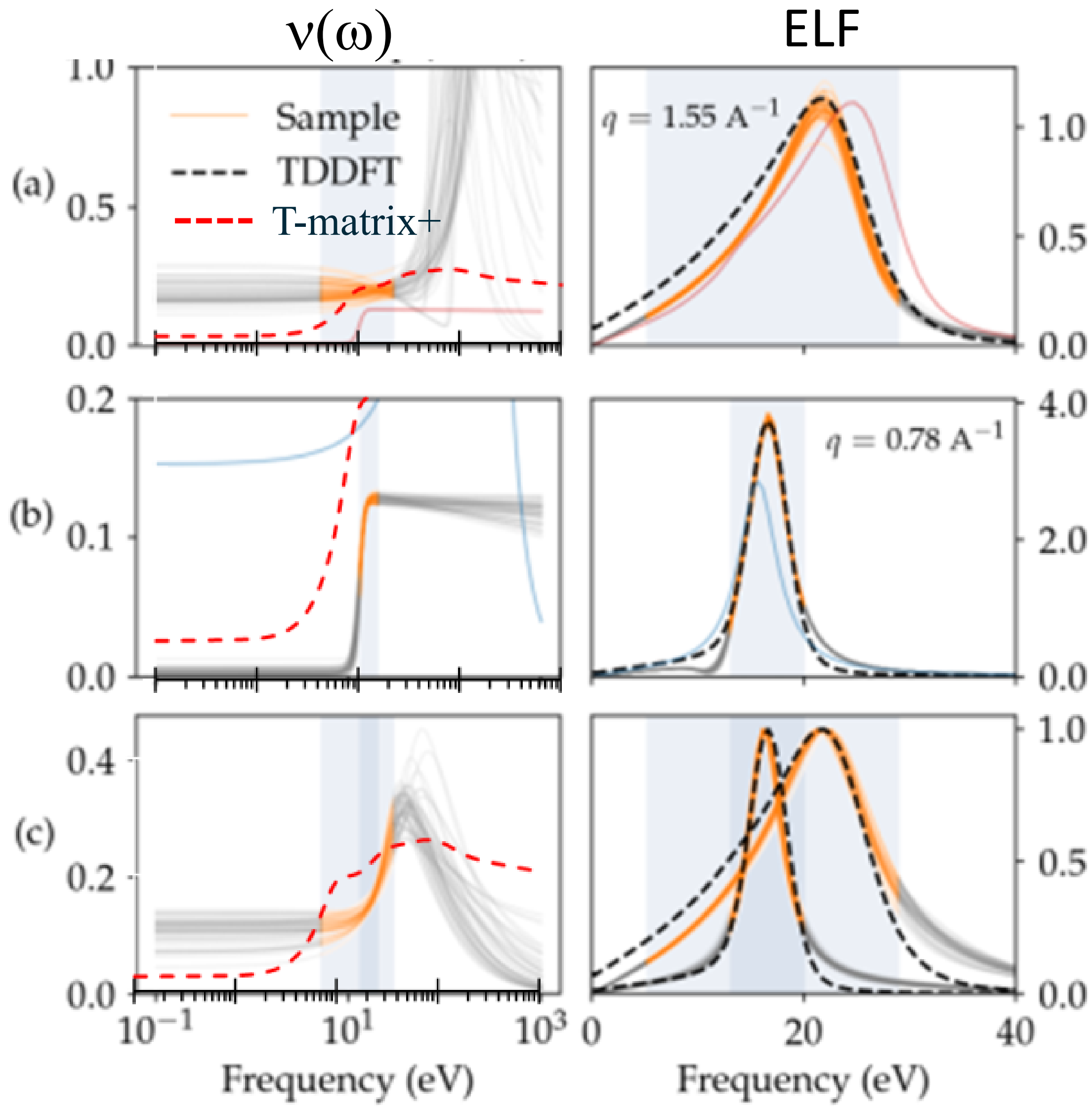
A range of ν(ω) – *different from our best ν(ω) model* – give reasonable fits to the ELF from time-dependent density functional theory (TDDFT)

Fitting to TDDFT data at a smaller angle, we find an entirely different range of plausible ν(ω)

Applying a typical ν(ω) from one angle to the other modestly degrades the fit to both ELFs

A simultaneous fit of ELFs at both angles restores good agreement with a ν(ω) that is closer to our best model

The DC limit remains ill-constrained



Conclusions

- Given a realistic XRTS spectrum from a well characterized sample, Bayesian inference with Markov-chain Monte Carlo sampling can roughly recover values of $\nu(\omega)$ at frequencies near the signal peak, but not at the DC limit

- Data at multiple angles improve constraints on $\nu(\omega)$ over larger frequency ranges

- For $\nu(0)$/DC conductivities, direct measurements at lower frequencies may be necessary (see THz measurements from Ofori-Okai et al)