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Statistical inference of electron-ion collision rates from simulated XRTS data

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Electron-ion collision frequencies inform the (free) electron response to an external perturbation

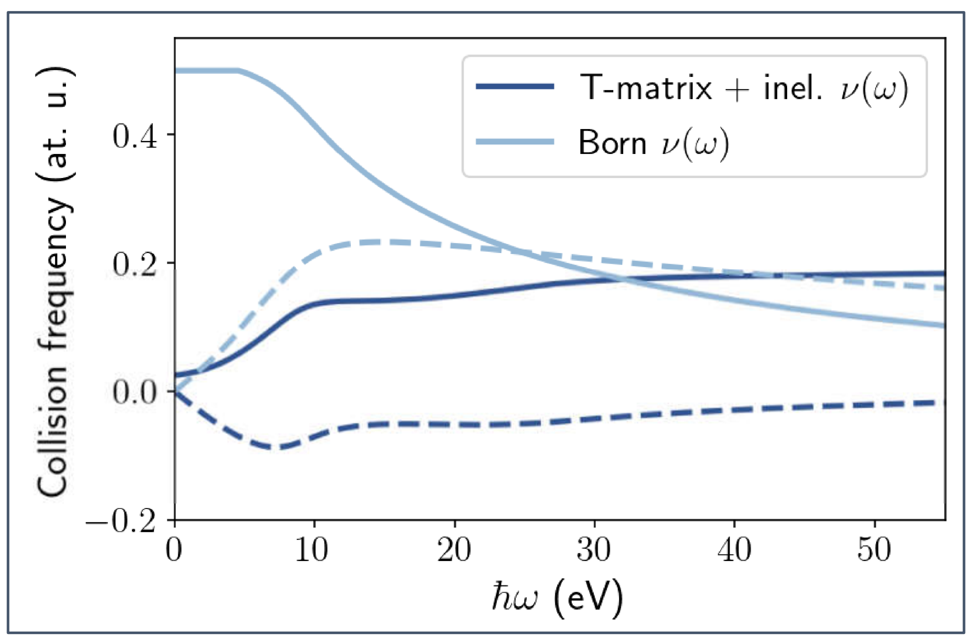
- e-i collision frequencies, $\nu(\omega)$, are important for
  - Modifying UEG dielectric theories (dynamic structure factors, stopping powers, etc.)
  - Plasma/MHD simulations
  - Conductivities - specifically, the DC components are related:

$$\sigma(\omega = 0) = n_e / \nu(\omega = 0)$$

- Currently, e-i collision rate/frequency theories are indirectly validated against x-ray Thomson scatterting (XRTS) spectra

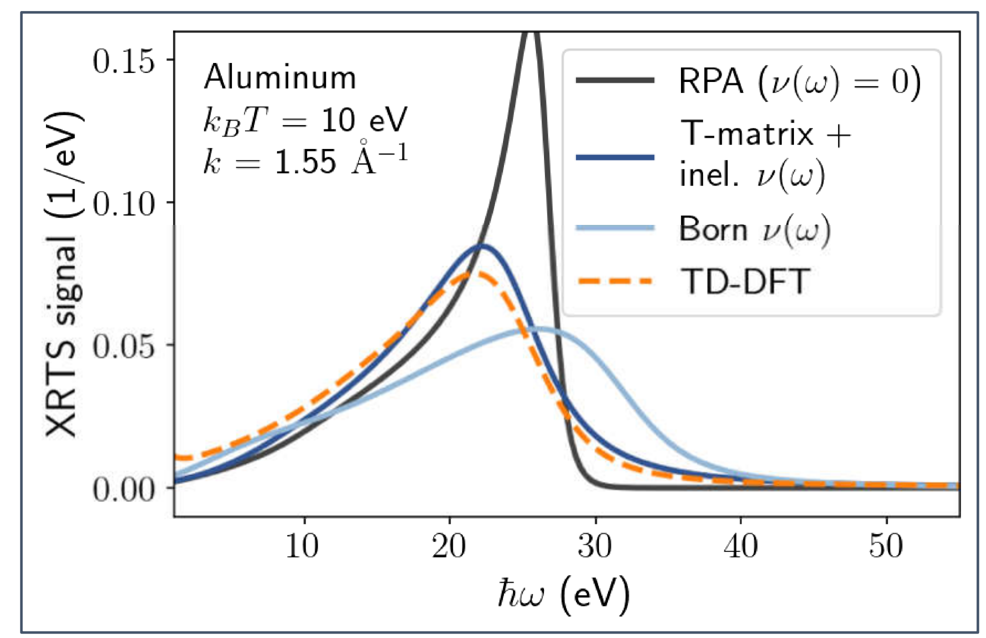
Modeling XRTS spectra with collisions

- Use a *modified* **Mermin** model to simulate XRTS scattering spectra
  - Modified = non-ideal density of states
  - Depends on the **electron-ion collision frequency, $\nu(\omega)$**



Mermin($\nu(\omega)$)

forward evaluation



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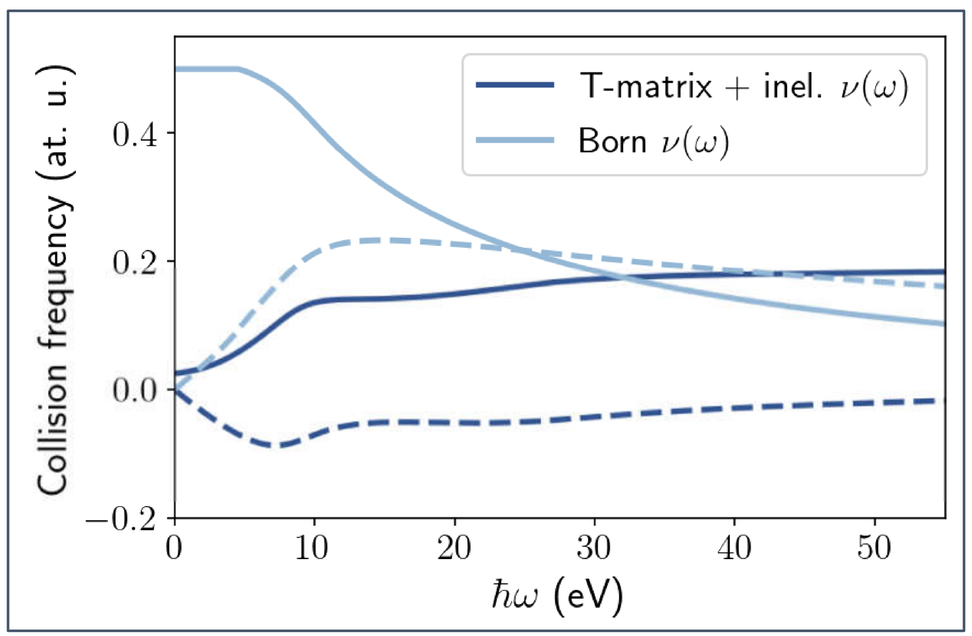

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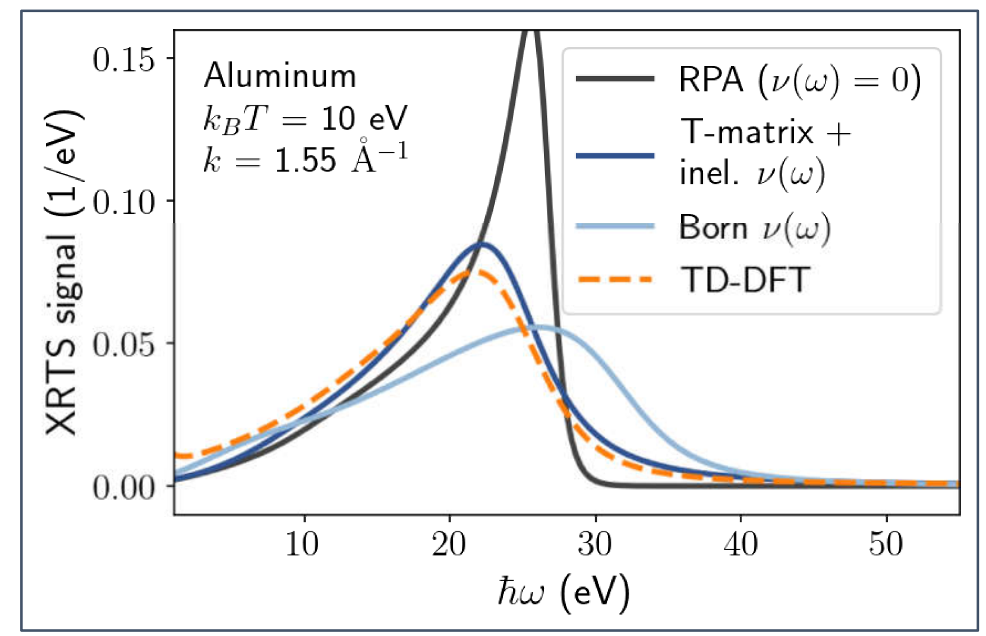


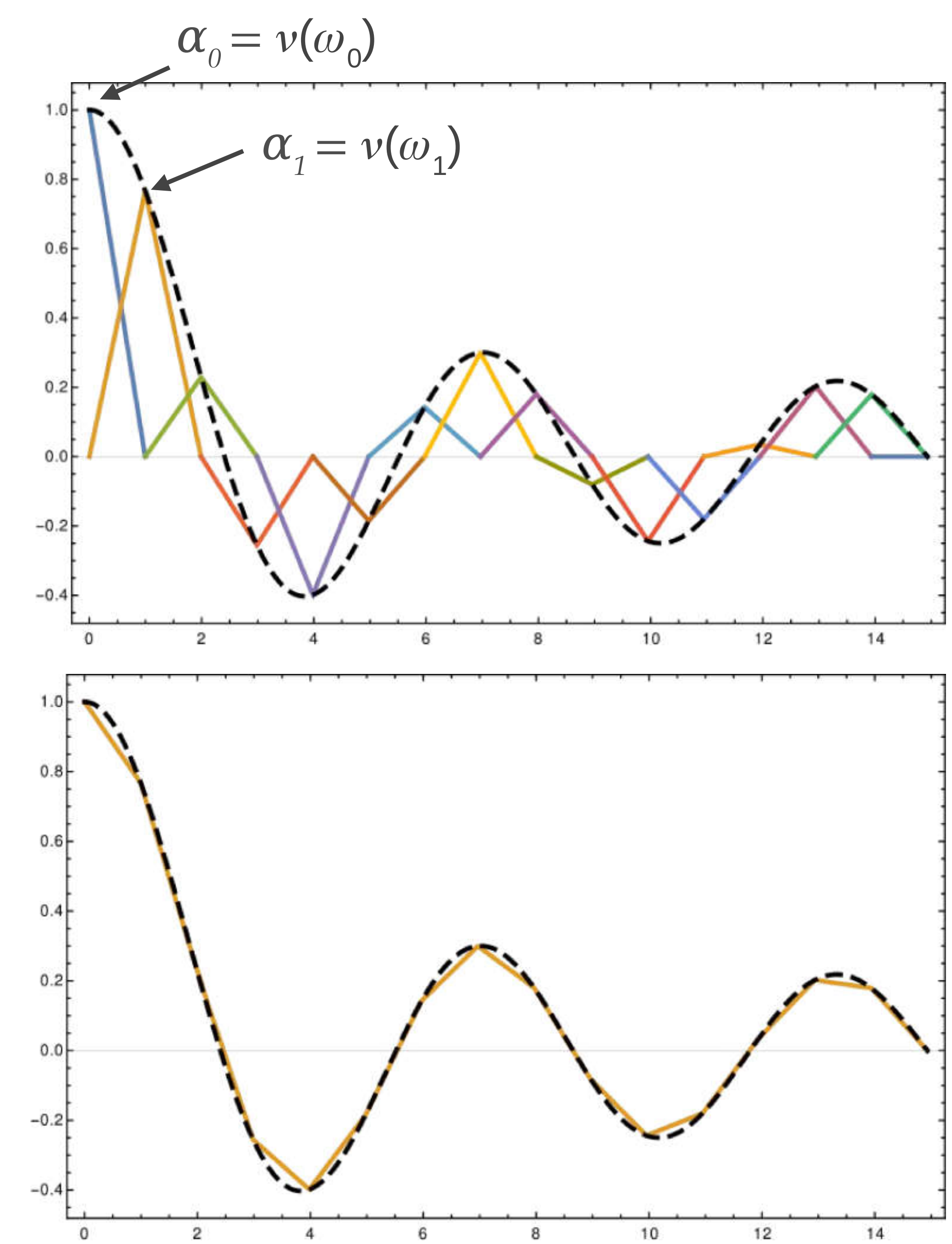
Can we infer dynamic collision frequencies from XRTS spectra?

Simplify problem by parametrizing $\nu(\omega)$

- Want representation be as general as possible:
  - Parametrize $\nu(\omega)$ with (unit) triangle basis functions

$$\nu(\omega) = \sum_{i=0}^{p} \alpha_i \mathrm{tri}_i(\omega)$$

- Equivalent to linear interpolation with p points ($\nu(\omega_i) = \alpha_i$)
- ex.: Bessel function with p=16

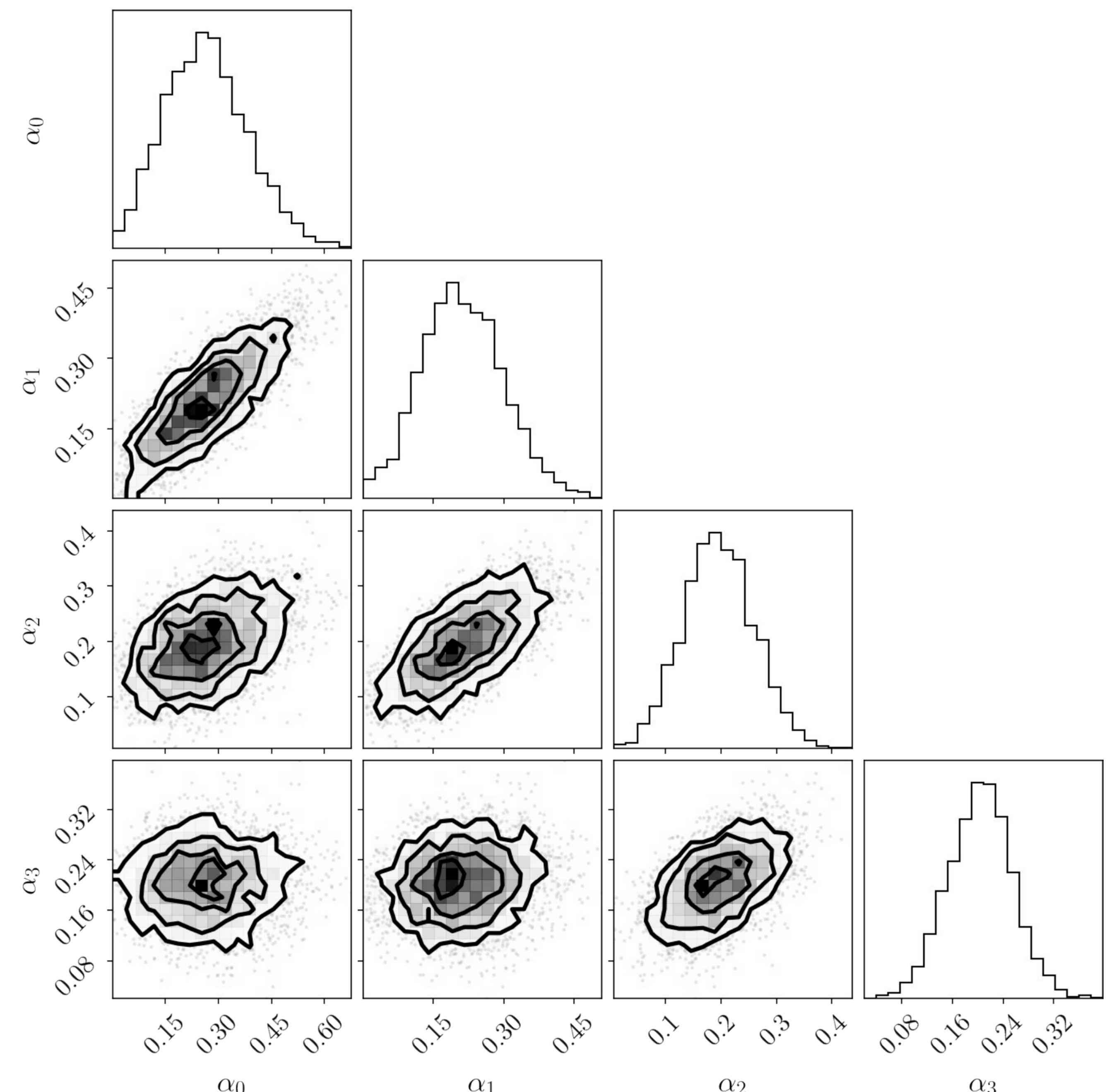


Statistical approach to inferring $\nu(\omega)$

- Optimization-based inversion to find $\alpha_i \, (= \nu(\omega_i))$ is unstable [2]
- Consider the *posterior* distribution of parameters, $\boldsymbol{\alpha}$, given XRTS data, $\boldsymbol{y}$:

$$\underbrace{p(\alpha|y)}_{\text{posterior}} \propto \underbrace{p(y|\alpha)}_{\text{likelihood}} \, \underbrace{p(\alpha)}_{\text{prior}}$$

- Markov Chain Monte Carlo (MCMC) to sample from high-dimensional posterior (using emcee package [3,4])

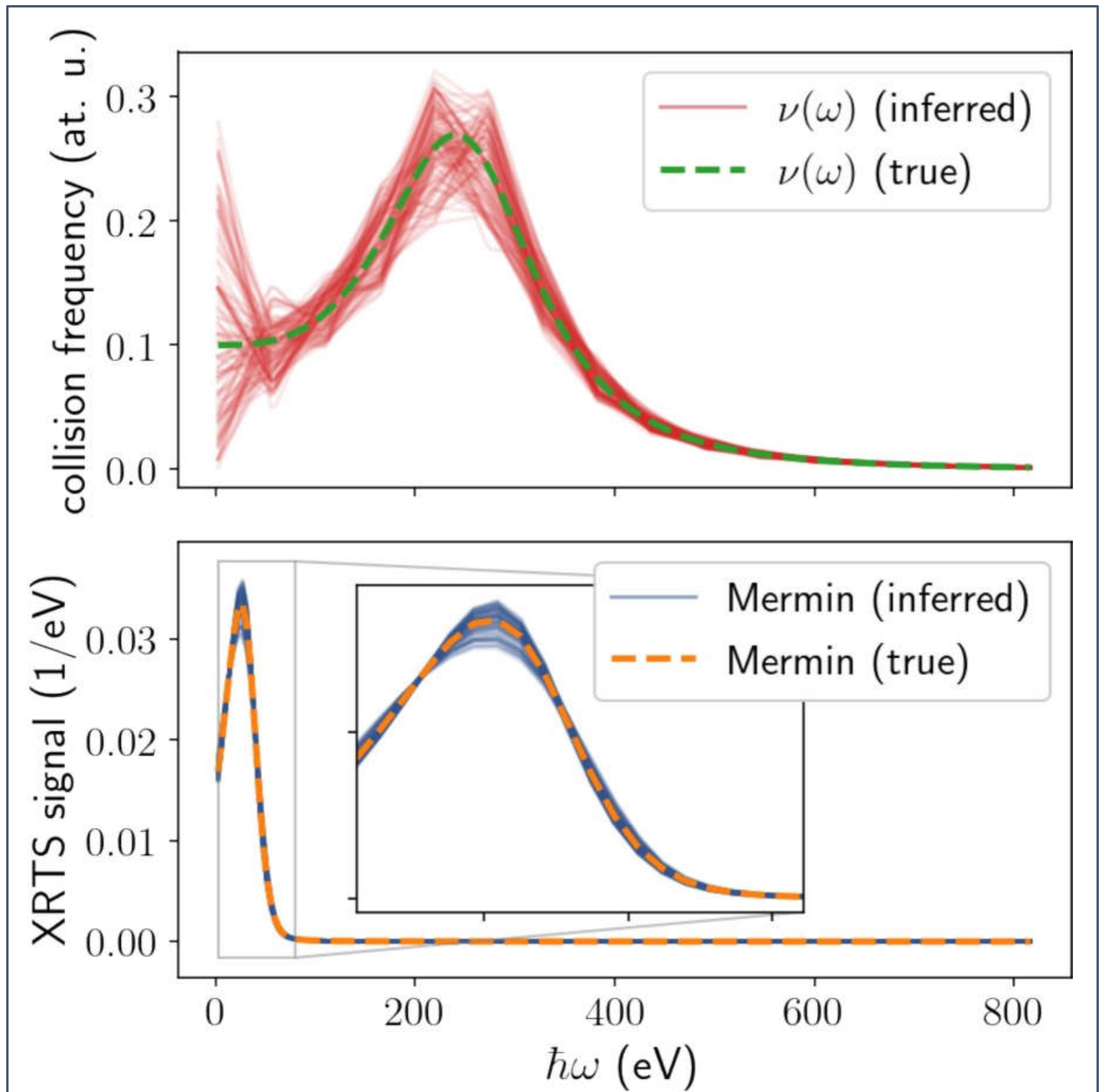


[2] M. F. Kasim *et al.*, *Phys. Plasmas* **26**, 112706 (2019)

[3] D. Foreman-Mckey *et al.*, *Astro. Soc. of the Pacific* **125**, 925 (2013)

[4] D. Foreman-Mckey, *J. Open Source Software* **1**, 2 (2016)

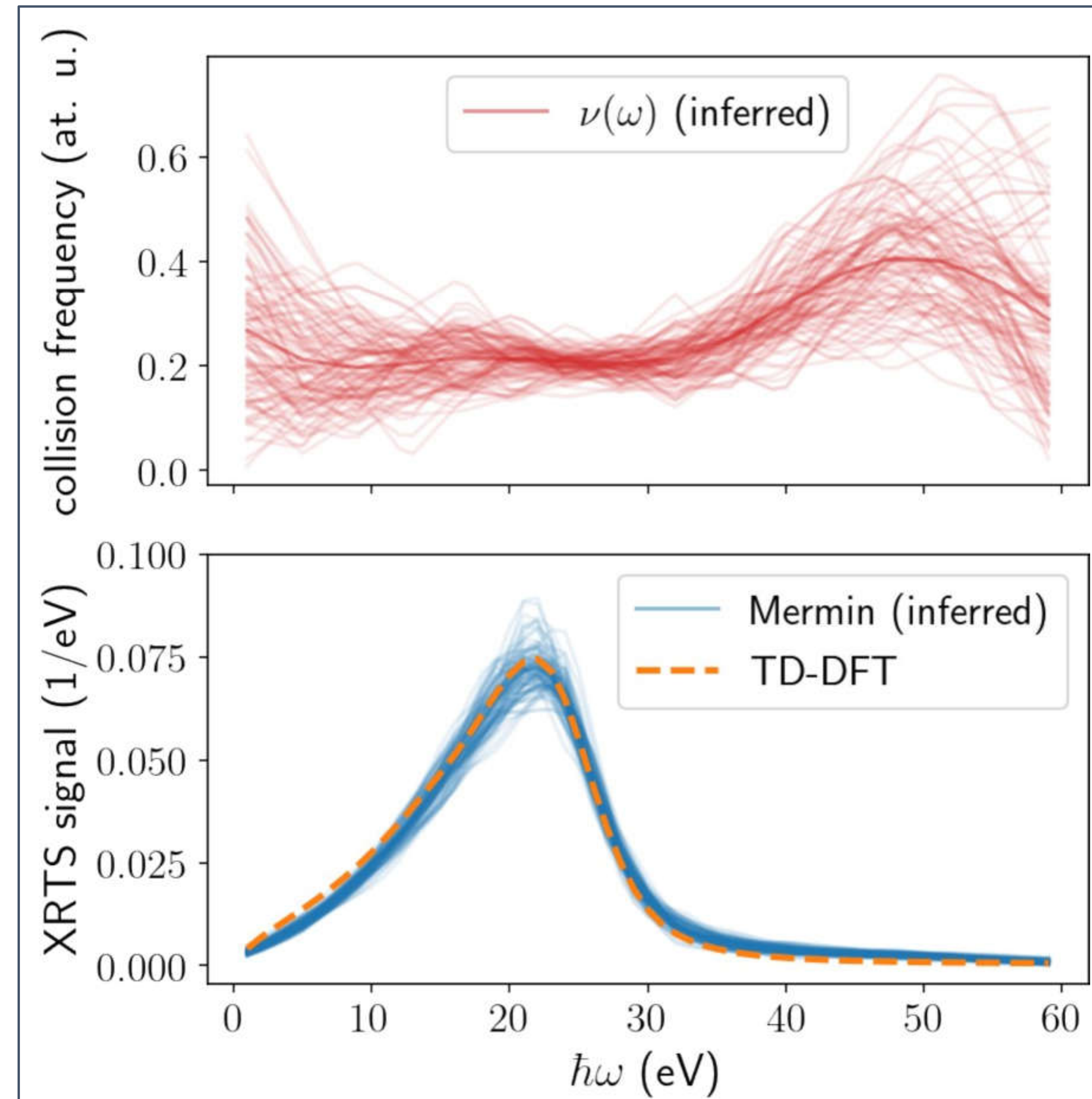
Test case: inference with known collision rates



- Using only the input XRTS data, we sample from the posterior distributions of parameters to infer $\nu(\omega)$
- Multiple $\nu(\omega)$ yield similar DSFs
  - Not surprising!

Inferring collision rates from simulated XRTS

- Even with a flexible model for $\nu(\omega)$, unable to perfectly fit the TD-DFT XRTS signal
- A "good fit" to the plasmon peak does not constrain the shape of the collision frequency
  - Not confident in low- and high-energy limits

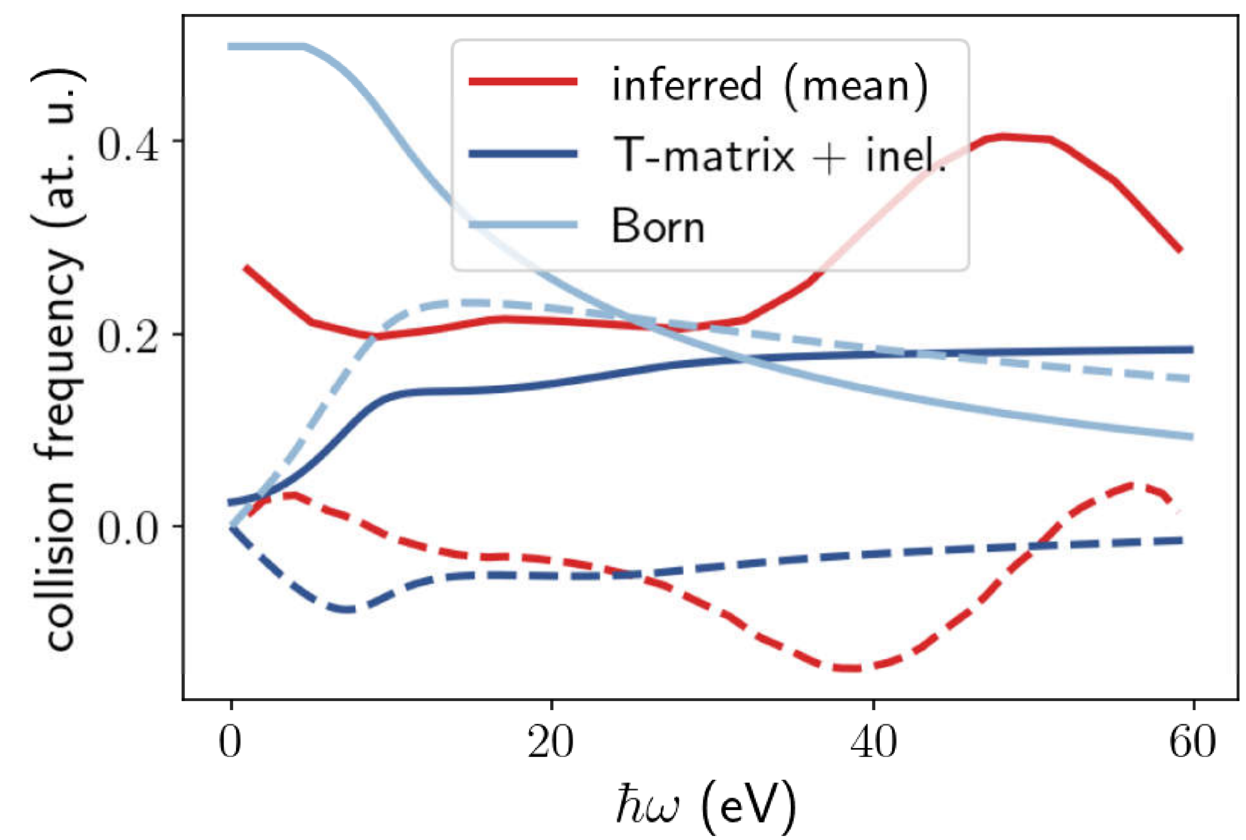


Conclusions

- Using a statistical approach for inference, we are finding that XRTS spectra do not fully constrain collision frequencies through the Mermin model
- However, the constrained portions of $\nu(\omega)$ can help validate collision rate theories in WDM

Drawbacks:

- Method is only meaningful insofar as the Mermin model is physically correct
- Exploring high-dimensional spaces is time consuming!



Acknowledgments

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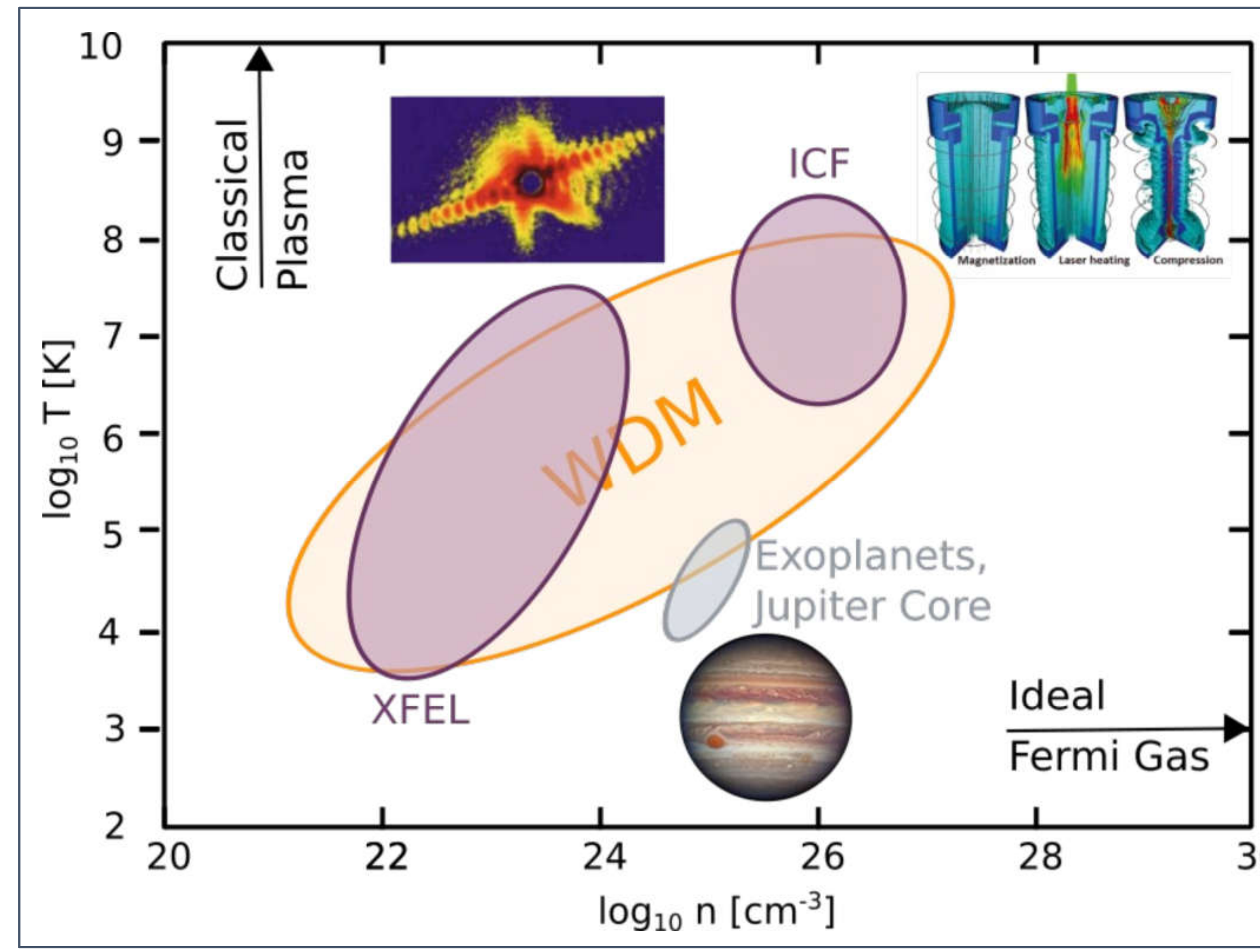
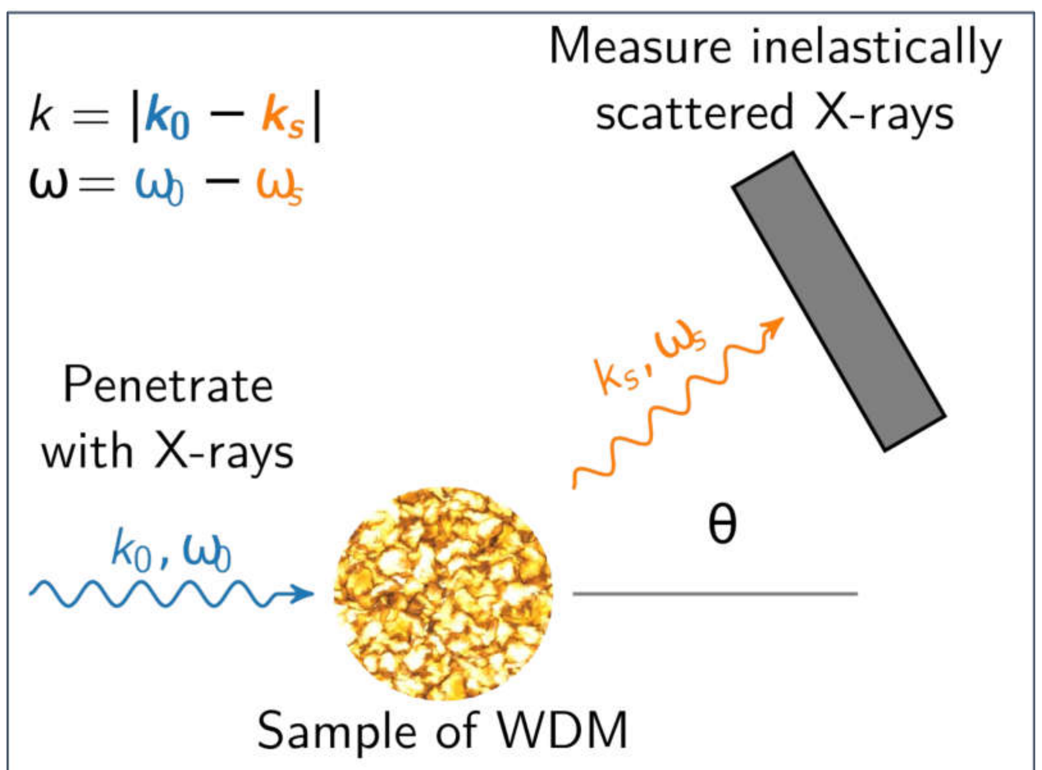
Background

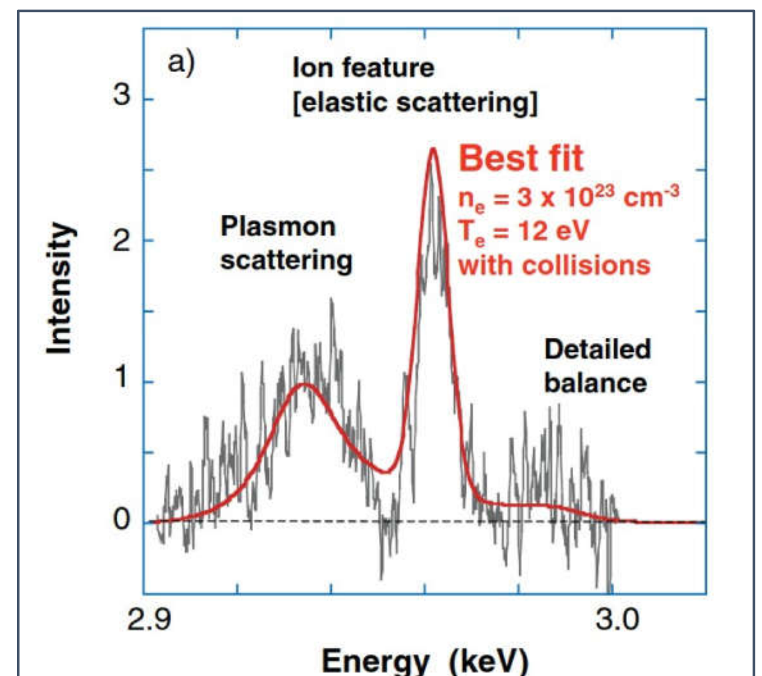
- Warm dense matter (WDM; near-solid densities, thermal energies ≳ 1 eV, or 11,604 K) exists in planetary cores and is created in inertial confinement fusion experiments



Background

- X-ray Thomson scattering (XRTS) can probe laboratory warm dense matter (WDM) samples
- Sample conditions are inferred from comparisons of XRTS data with complex model predictions



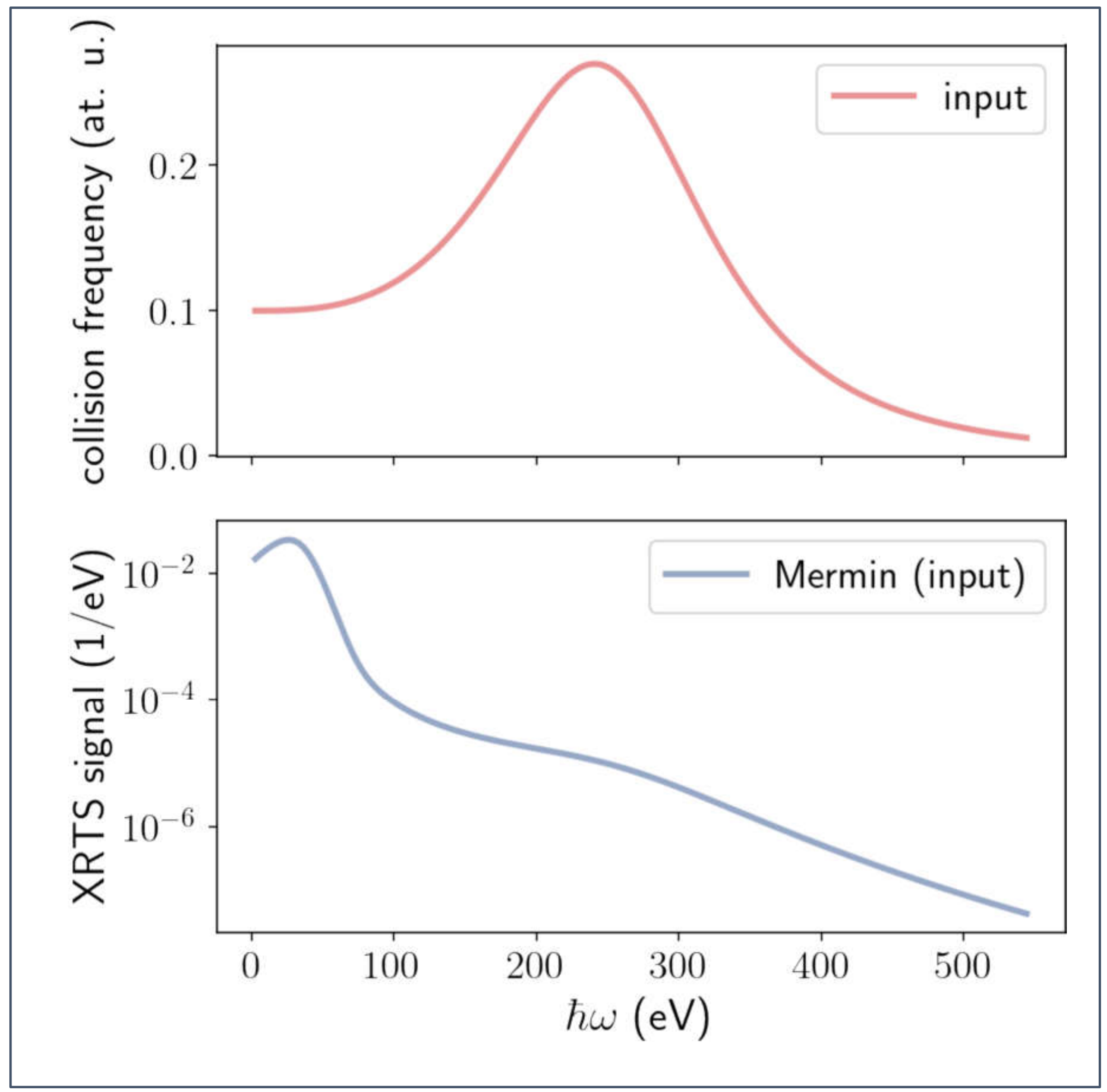


XRTS spectra [1].

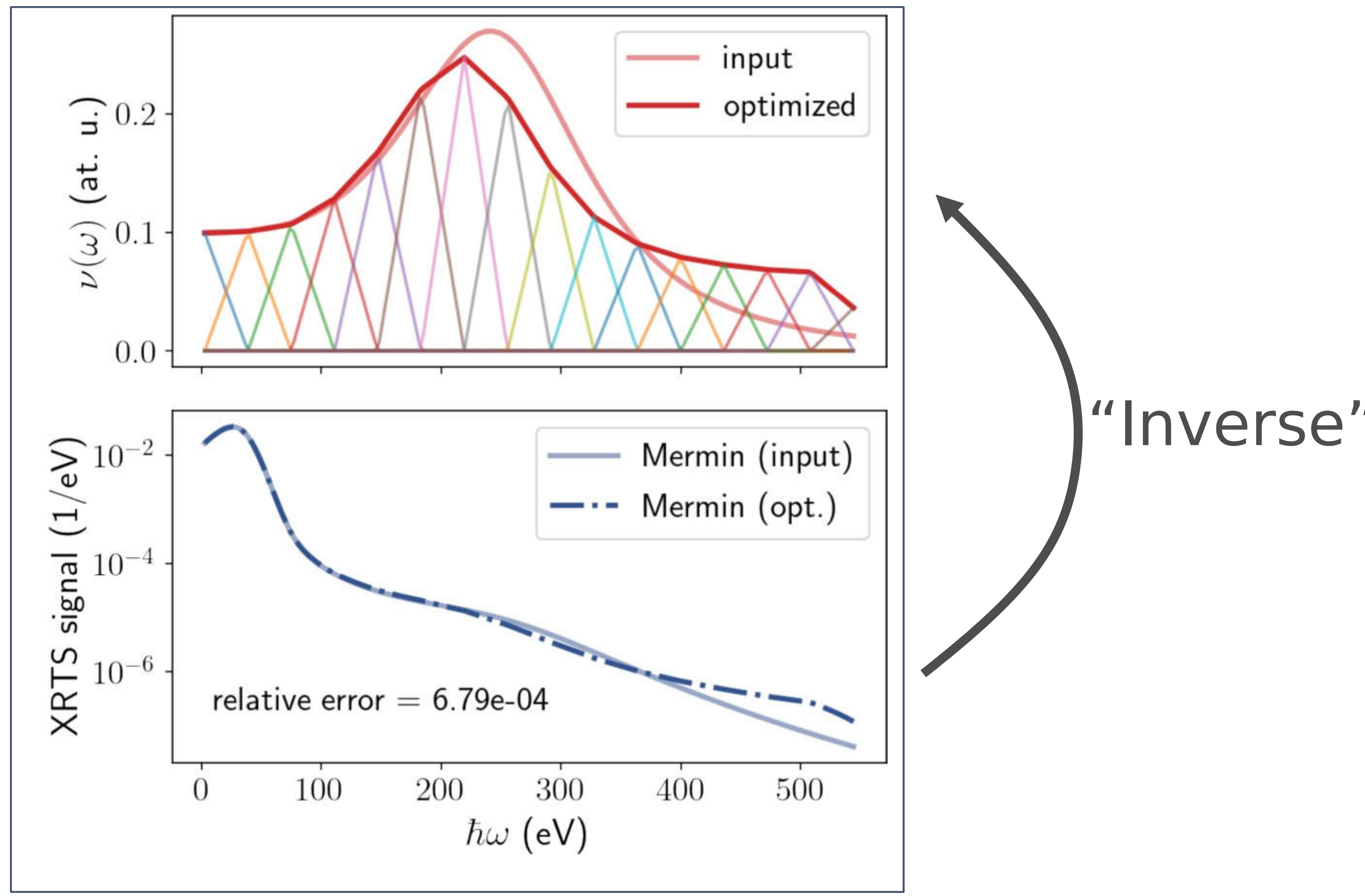
[1] S. H. Glenzer *et al.*, *Phys. Rev. Letters* **98**, 065002 (2007)

Optimize to find α_i

Forward



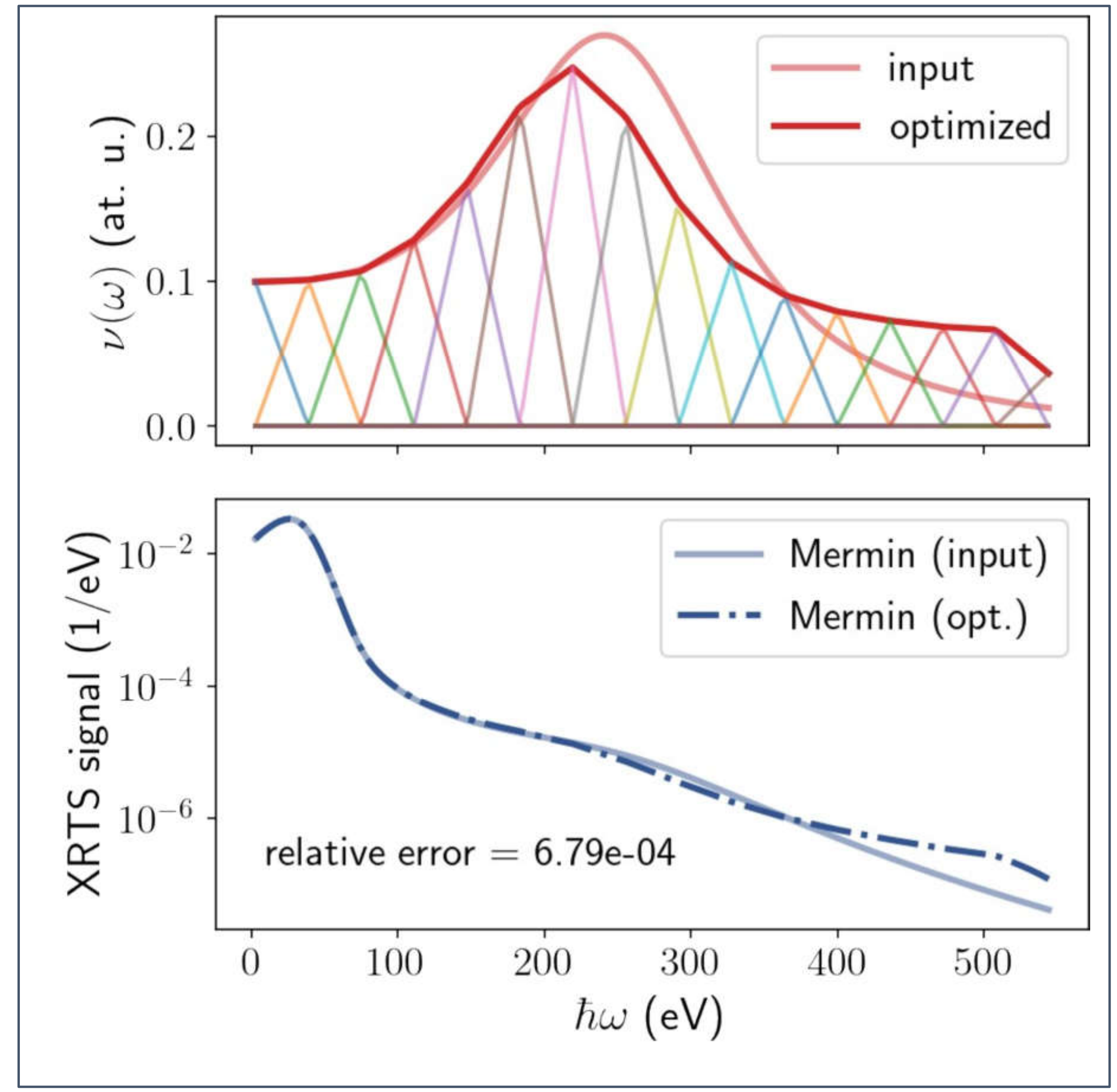
Optimize to find α_i



Optimization is unstable!

- **Inversion problem instabilities**: different $\nu(\omega)$ lead to roughly similar XRTS spectra [2]
- Can we explore possible collision frequencies that yield outcomes that agree with XRTS data within some *relative* uncertainty range?

$$\nu(\omega) = \sum_{i=0}^{p} \alpha_i \mathrm{tri}_i(\omega)$$



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