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Estimating ionization states and continuum lowering from *ab initio* path integral Monte Carlo simulations for warm dense hydrogen

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Warm dense matter (WDM), prevalent in astrophysical objects and crucial for inertial confinement fusion (ICF), presents significant challenges in characterizing fundamental properties such as ionization degree and continuum lowering. Experimental diagnostics of WDM, particularly for hydrogen due to its low scattering cross-section, are limited and often rely on model-dependent analyses, complicating the development and validation of equation of state (EOS) tables. While ab initio methods like path integral Monte Carlo (PIMC) simulations offer exact descriptions, direct access to ionization degree and continuum lowering is not inherent to these methods [1] and often is highly dependent on a chosen definition.

Here, we present a novel approach to extracting ionization potential depression (IPD) and ionization degree from exact ab initio PIMC simulations of warm dense hydrogen by applying a chemical model based on the Chihara decomposition, which treats bound and free electrons separately. This allows for a definition of the ionization state as the mean number of free electrons per nucleus and IPD as the effective reduction in electron binding energy due to plasma interactions. In contrast to experimental approaches that grapple with noise, non-equilibrium effects, and source-instrument function convolutions, our method involves forward-fitting a chemical dynamic structure factor (DSF) to the imaginary-time correlation function (ITCF) obtained from PIMC simulations at well-defined thermodynamic conditions [2].

By separately analyzing the elastic (Rayleigh weight) and inelastic components of the scattering signal within the Chihara framework, we extract best-fit parameters for ionization and IPD over an extended range of scattering wave vectors, mimicking various scattering angles accessible in x-ray Thomson scattering (XRTS) experiments. Comparisons with commonly used models for ionization reveal qualitative agreement but also deviations, particularly at high densities and temperatures. We also investigate the sensitivity of the dynamic structure factor to ionization and continuum lowering as a function of the scattering angle, providing important implications for the design and interpretation of future XRTS experiments. Notably, we observe a decreasing sensitivity of the inelastic component to both ionization and IPD at increasing scattering angles, suggesting limitations in extracting these parameters from non-collective scattering regimes.

Further, this approach allows us to qualitatively investigate the effects of ionization degree and IPD in the imaginary-time domain. By bridging the gap between exact ab initio simulations and chemical model interpretations, our approach offers a valuable tool for benchmarking theoretical models, informing the development of accurate EOS tables for high energy density matter, and guiding the design of future experimental campaigns at facilities like the European XFEL and LCLS.

References

[1] M. Bonitz et al., Phys. Plasmas 31 (2024)

[2] T. Dornheim et al., Nat. Commun. 13 (2022)

[3] H. Bellenbaum et al., arXiv:2503.14014v1 [physics.chem-ph]

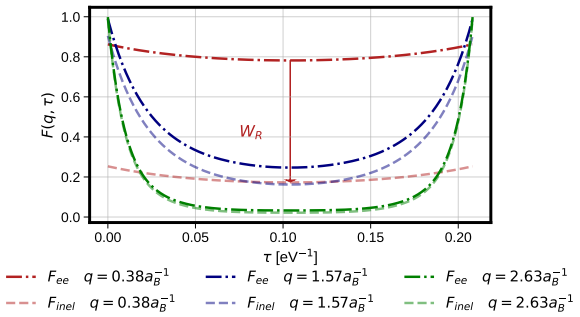

Fig. 1: ITCF split into elastic (WR) and inelastic contributions for different scattering vectors q.