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Estimating ionization degree 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. *Ab initio* methods like path integral Monte Carlo (PIMC) offer exact simulations but do not inherently provide direct access to these quantities.

We introduce a method to extract ionization potential depression (IPD) and ionization degree from PIMC simulations using a chemical model based on Chihara decomposition, which separates bound and free electron contributions. By forward-fitting a chemically informed dynamic structure factor to the imaginary-time correlation function obtained from PIMC, we retrieve best-fit estimates for both IPD and ionization degree under well-defined thermodynamic conditions.

This approach enables the analysis of elastic and inelastic scattering components across a range of wave vectors, allowing us to assess the sensitivity of scattering signals to ionization and IPD. We find that sensitivity decreases at higher scattering angles, suggesting limitations in extracting these properties in non-collective regimes. By bridging exact simulations and chemical models, this method supports equation-of-state development and informs the design of future x-ray Thomson scattering experiments.

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