From the imaginary time to real-world experiments

Understanding electronic correlations in warm dense matter: from *ab initio* simulations to experiments

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In Short

- Warm dense matter (WDM) is an extreme state characterized by high temperatures ($T \sim 10^3 - 10^8$ K) and densities even exceeding ordinary solids
- WDM naturally occurs in astrophysical objects (e.g. giant planet interiors, brown dwarfs, neutron stars)
- WDM is of high importance for technologies such as inertial confinement fusion
- Diagnostics of experiments with WDM are challenging and require theoretical modeling
- We explore novel *ab initio* path integral Monte Carlo (PIMC) simulations of WDM and present exact results for conditions realized e.g. at the National Ignition Facility (NIF)

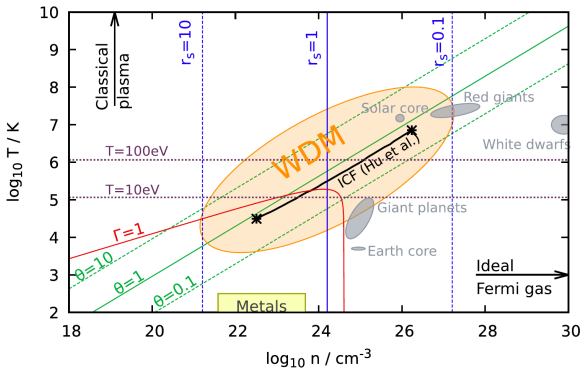

***Figure 1:** Warm dense matter (WDM) parameters (orange bubble) in the density-temperature plane. The grey objects indicate conditions in various astrophysical objects. Also shown are lines of constant density parameter (Wigner-Seitz radius) $r_s = d/a_\mathrm{B}$, degeneracy temperature $\Theta = k_\mathrm{B}T/E_\mathrm{F}$ (with E_F being the Fermi energy), and classical coupling parameter Γ. Taken from Dornheim* et al. *[1].*

Over the last years, there has emerged a remarkable interest in the properties of matter at extreme densities and temperatures. Of particular importance is so-called *warm dense matter* (WDM), an extreme state that is characterized by high temperatures ($T \sim 10^3 - 10^8$ K) and densities partially exceeding the density of ordinary solids; see Fig. 1 for an overview plot. From a physical perspective, these conditions are quite ubiquitous throughout our universe and naturally occur in astrophysical objects such as giant planet interiors and brown dwarfs. In addition, WDM is important for state-of-the-art technological developments. For example, the fuel capsule in a typical inertial confinement fusion (ICF) experiment has to traverse the WDM regime in a controlled way to reach ignition.

As a consequence of this remarkable interest, WDM is nowadays routinely realized at large research facilities around the globe such as the European XFEL in Germany or the National Ignition Facility in the USA [2]. A major challenge is given by the accurate diagnostics. Often, even basic parameters such as the temperature or the density cannot be directly measured, and have to be inferred indirectly from other observations. In this context, the x-ray Thomson scattering (XRTS) technique [3,4] has emerged as a very import method to diagnose the thermodynamic state of a given system. On the one hand, XRTS measurements allow one in principle to infer a number of system parameters that are relevant for example for equation-of-state tables—a key input to astrophysical models, the modeling of fusion experiments, etc. On the other hand, the thus inferred parameters can strongly depend on the employed model, which are usually based on a number of de-facto uncontrolled approximations.

This unsatisfactory situation is a direct consequence of the notorious difficulty to find an accurate theoretical description of WDM [5]. Indeed, a true *ab initio* approach to WDM must have the capability to take into account the intriguingly intricate interplay of a variety of physical effects, including Coulomb coupling, quantum degeneracy, and strong thermal excitations.

In this project, we carry out unprecedented *ab initio* path integral Monte Carlo (PIMC) simulations of a variety of low-Z elements in the WDM regime. Our simulations are not based on the usual fixed-node approximation to deal with the fermion sign problem [6]; therefore, they are computationally expensive, but exact within the given error bars. Moreover, the absence of any nodal restriction gives us access to the full imaginary-time structure of the system. First, we have shown that different imaginary-time correlation functions (ITCF) give one access to a number of linear and nonlinear response properties of a given system [1]. Second, such ITCFs constitute the basis for an *analytic continuation* to reconstruct dynamic properties such as the dynamic structure

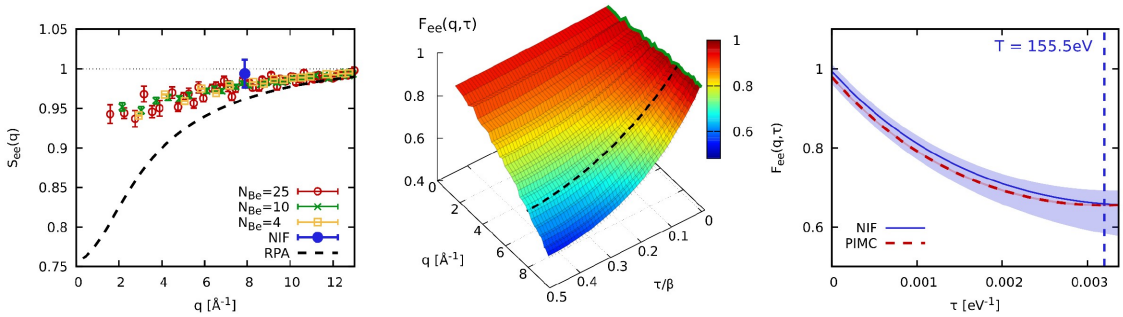

Figure 2: *PIMC simulation of the XRTS experiment with warm dense beryllium carried out at the NIF by Döppner* et al. *[2]. Left: electronic static structure factor $S_{ee}(\mathbf{q})$; center: full ITCF as a function of the imaginary time τ and wave number q; right: experimentally observed ITCF along the τ-direction.*

factor $S(\mathbf{q},\omega)$—a key property for the modeling of XRTS experiments. Third, it is straightforward to obtain the ITCF directly from XRTS measurements, which has a number of key advantages.

Very recently, we have shown that analyzing XRTS experiments in the imaginary-time domain gives one direct access to parameters such as the temperature T [7] and the electronic static structure factor $S_{ee}(\mathbf{q})$ [8]. Moreover, working in the imaginary time allows us to directly compare our exact PIMC simulations with the experimental observation. In Fig. 2, we compare new PIMC simulations of warm dense beryllium to the recent XRTS experiment at NIF by Döppner *et al.* [2]. Evidently, our results are in excellent agreement with the experiment. This gives us the unprecedented capability to predict the outcome of XRTS measurements on WDM with high precision, which is a game changer for the study of matter under extreme conditions.

Direct applications of our work include the interpretation of XRTS experiments by inferring hitherto approximated parameters such as the density or the charge state. Moreover, we can guide the development of new experimental setups by carrying out sensitivity studies with respect to various parameters of interest. Finally, we will use our new PIMC results to unambiguously benchmark density functional theory (DFT), which currently constitutes the work horse of WDM theory. All simulation results will be made openly available, and can be freely used by the community for other applications.

WWW

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More Information

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Project Partners

Dr. T. Döppner, National Ignition Facility at the Lawrence Livermore National Laboratory, USA

Funding

ERC Starting Grant "Predicting the Extreme" (agreement no 101076233)
DFG Research Grant "Radiation transport in dense hydrogen plasmas at conditions relevant to the interiors of Red Dwarfs" (project no 495324226)

DFG Subject Area

308-32