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Understanding electronic correlations in warm dense quantum plasmas

Warm dense matter (WDM)—an extreme state that is characterized by extreme densities and temperatures—has emerged as one of the most active frontiers in plasma physics and material science. In nature, WDM occurs in astrophysical objects such as giant planet interiors and brown dwarfs. In addition, WDM is highly important for cutting-edge technological applications such as inertial confinement fusion and the discovery of novel materials. In the laboratory, WDM is studied experimentally in large facilities around the globe, and new techniques have facilitated unprecedented insights. Yet, the interpretation of these experiments requires a reliable diagnostics based on accurate theoretical modeling, which is a notoriously difficult task [1].

In this work, I will give an overview of how we can use exact ab-initio path integral Monte Carlo (PIMC) simulations [2] together with thermal density functional theory (DFT) calculations to get new insights into the behavior of WDM. Moreover, I will show how switching to the imaginary- time representation allows us to significantly improve the interpretation of X-ray Thomson scattering (XRTS) experiments, which are a key diagnostic for WDM [3]. Specifically, I will present a model-free temperature diagnostic [4] based on the well-known principle of detailed balance, but available for all wave numbers, and a new idea to directly extract the electron—electron static structure factor from an XRTS measurement [5]. As an outlook, I will show how new PIMC capabilities will allow to give us novel insights into electronic correlations in warm dense quantum plasmas, leading to unprecedented agreement between experiments [6] and theory.

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[2] M. Böhme et al., Physical Review Letters 129, 066402 (2022)
[3] S. Glenzer and R. Redmer, Reviews of Modern Physics 81, 1625 (2009)
[4] T. Dornheim et al., Nature Communications 13, 7911 (2022)
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