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Ab Initio Path Integral Monte Carlo Results for the Dynamic and Static Density Response of Correlated Electrons: From the Electron Liquid to Warm Dense Matter

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Over the last decades, there has emerged a growing interest in warm dense matter (WDM), an exotic state with extreme densities and temperatures. These conditions are relevant for the description of astrophysical objects, laser-excited solids, and the pathway to inertial confinement fusion. Despite the remarkable experimental progress at large research facilities around the globe, a thorough theoretical description of WDM is notoriously difficult due to the complicated interplay of (1) Coulomb coupling, (2) thermal excitations, and (3) quantum degeneracy effects.

In this work, we focus on the uniform electron gas (UEG), one of the most fundamental model systems in physics and quantum chemistry. Although most ground state properties of the UEG have been known for decades, a full thermodynamic description at WDM conditions has only been achieved recently [1] on the basis of ab initio quantum Monte Carlo simulations [2,3]. In this contribution, we extend these considerations to the dynamic structure factor---the key quantity in X-ray Thomson scattering (XRTS) experiments, which have emerged as a standard tool of diagnostics in WDM experiments.

More specifically, we have carried out extensive path integral Monte Carlo simulations of the UEG going from WDM conditions to the strongly correlated electron liquid regime to compute an imaginary-time density—density correlation function. The latter is subsequently used as input for a new reconstruction procedure, which allows to obtain ab initio results for the dynamic structure factor including all exchange-correlation effects [4,5]. This has allowed us to compute the first accurate data for the dynamic structure factor for different densities and temperatures, and to gauge the accuracy of previous approximations. Interestingly, at strong coupling we find nontrivial shapes around intermediate wave vectors, which manifest in a negative dispersion relation.

Moreover, we present extensive new results for the static local field correction, which is of high importance as input for, e.g., quantum hydrodynamics, electrical and thermal conductivities, advanced XC-functionals for DFT, and the interpretation of experiments. In summary, we demonstrate that accurate path integral Monte Carlo results for the UEG constitute a key component to WDM theory and are highly needed to put existing methods on a more reliable footing.

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