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Quantum Monte Carlo Simulation of Warm Dense Matter

Tuesday 22 February 2022 14:00 (30 minutes)

Warm dense matter is of high current interest for many applications, including astrophysics, material science, and fusion research. Yet, the accurate description of electronic correlation effects at these conditions is most difficult, and often computationally intensive ab-initio methods have to be used [1]. The most accurate approach is given by the quantum Monte Carlo (QMC) technique, which is, in principle, capable to give one exact results for the full quantum many-body problem of interest without any empirical input. Consequently, parametrizations of accurate QMC data constitute the basis for a gamut of applications, such as the construction of XC-functionals for density functional theory (DFT).

In this talk, I focus on the electronic density response of WDM to an external perturbation, which is of central interest for WDM theory, such as the interpretation of X-ray Thomson scattering (XRTS) experiments and the construction of advanced XC-functionals for DFT. In particular, I will show how we can use the ab-initio path integral Monte Carlo (PIMC) method to estimate the exact density response to an external harmonic perturbation. First and foremost, this allows us to compute the electronic XC-kernel (also known as local field correction in the context of dielectric theory), which has recently become available as a neural-net representation [2] for a uniform electron gas. Secondly, I will show how our imaginary-time PIMC data can be used as a starting point for an analytic continuation [3]. This gives us access to the dynamic structure factor, which is the key property in XRTS experiments. Lastly, I will talk about nonlinear effects in WDM [4], which cannot be neglected in many situations of experimental relevance.

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[2] T. Dornheim, J. Vorberger, S. Groth, N. Hoffmann, Z. Moldabekov, and M. Bonitz, J. Chem. Phys. 151, 194104 (2019)
[3] T. Dornheim, S. Groth, J. Vorberger, and M. Bonitz, Phys. Rev. Lett. 121, 255001 (2018)
[4] T. Dornheim, J. Vorberger, and M. Bonitz, Phys. Rev. Lett. 125, 085001 (2020)

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