

Recent progress in simulations of dense quantum plasmas

and warm dense matter

M. Bonitz¹, P. Hamann¹, T. Dornheim², Z. Moldabekov², A. Filinov¹, and J. Vorberger³

¹Institute for Theoretical Physics and Astrophysics, Kiel University, ²Center for Advanced Systems Understanding, Görlitz, ³Helmholtz-Zentrum Dresden-Rossendorf e-mail (speaker): bonitz@physik.uni-kiel.de

Presently we are witnessing dramatic progress in experiments with dense quantum plasmas where matter is being compressed to densities exceeding solid density. At the same time, accurate laser and x-ray based diagnostic tools have emerged that probe the properties of such warm dense matter. To understand these experiments and predict new ones poses a challenge to theory and simulations [1]. Promising tools include density functional theory (DFT), generalized quantum hydrodynamics (QHD), quantum kinetic equations (OKT, [2]), and quantum Monte Carlo (OMC, [3]). We will discuss some of the recent theory developments and present accurate results for the thermodynamic [4,5] and dynamic properties of the quantum electrons from QMC simulations, including the electron dynamic structure factor [6], dielectric function, plasmon dispersion [7], and momentum distribution [8]. We will also outline prospects of nonequilibrium simulations based on QKT [9, 10] and on OHD. For the latter we discuss how to improve the original equations to allow for reliable predictions [11, 12].



Figure: Schematic overview of computational methods for warm dense matter indicating their resolution of space and time scales. QBE: quantum Boltzmann equation, DFT: density functional theory, NEGF: nonequilbirium Green functions. From Ref. [1].

Warm dense matter is so complex that no single theory and simulation approach will be capable to describe all properties. Instead, a combination of methods that resolve small scales and accurately capture electronic correlations (but are computationally expansive) with coarse grained methods will be required to achieve predictive simulations in the future [1], as is sketched in the Figure.

References

- [1] M. Bonitz et al., Phys. Plasmas 27, 042710 (2020)
- [2] M. Bonitz, "Quantum Kinetic Theory", 2nd ed.
- Springer 2016

[3] T. Dornheim, S. Groth, and M. Bonitz, Phys. Reports **744**, 1-86 (2018)

- [4] T. Schoof et al., Phys. Rev. Lett. 115, 130402 (2015)
- [5] T. Dornheim *et al.*, Phys. Rev. Lett. **117**, 156403 (2016)
- [6] T. Dornheim *et al.*, Phys. Rev. Lett. **121**, 255001 (2018)
- [7] P. Hamann *et al.*, Contrib. Plasma Phys. **60**, e202000147 (2020)
- [8] K. Hunger et al., Phys. Rev. E 103, 053204 (2021)
- [9] N. Schlünzen *et al.*, J. Phys. Cond. Matt. **32** (10), 103001 (2020)
- [10] N. Schlünzen *et al.*, Phys. Rev. Lett. **124**, 076601(2020)
- [11] Zh. Moldabekov *et al.*, Phys. Plasmas 25, 031903(2018)
- [12] M. Bonitz et al., Phys. Plasmas 26, 090601 (2019)

This work is supported by the Deutsche

Forschungsgemeinschaft via grants BO1366-13 and BO1366-15 and by grant SHP 00026 for supercomputing time at the HLRN.