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Theoretical Foundations of Quantum hydrodynamics for dense plasmas

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Non-equilibrium processes are at the frontier of the high energy density plasma science. There are various methods for simulation of processes at different time scales and length scales. Such methods as time dependent DFT and method of Green functions are used for the description of such microscopic processes as the excitation and deexcitation of atoms, while a hydrodynamic simulation is the method of choice for the description of macroscopic instabilities such us Rayleigh Taylor. Various simulation methods of relevance for warm dense matter and dense plasmas and their approximate length and time scales are indicated qualitatively in Fig. 1. There is still a big gap between the length and time scale that are accessible by microscopic simulations and the scales that are relevant Quantum hydrodynamics (QHD) can serve as the missing link and can be a very useful tool that is complementary to other methods.

The talk will present microscopic theory of quantum hydrodynamics (MQHD), which goes beyond RPA by employing ab inito data for dynamic local field corrections [1,2]. Quantum hydrodynamic theory is presented as the orbital averaging of the MQHD equations. The range of applicability of QHD is analyzed. Going beyond the gradient expansion approximation, a fully non-local Bohm potential is derived [1,2].

Furthermore, the results for the dynamic structure factor of ions at dense plasma and WDM conditions will be presented [3, 4]. The applicability of the classical generalized hydrodynamics and of the QHD for the description of collective oscillations of ions are discussed. Additionally, the results for the energy loss characteristics of electrons at WDM and dense plasma conditions will be presented, where the static local field correction from ab initio QMC simulations [5] was used. Finally, the first results for the friction coefficient acting upon ions due to electrons will be reported, where friction represents a correction to the Born-Oppenheimer approximation within Langevin dynamics simulation of ions [6].

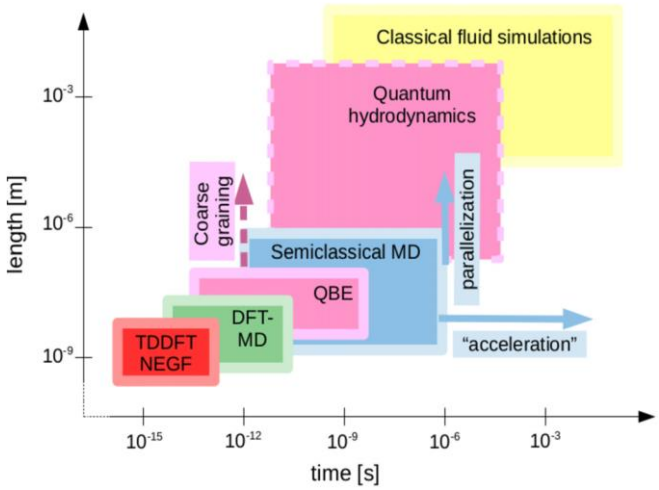

FIG. 1. Overview on the simulation methods of and quantum plasmas, and their approximate length and time scales. DFT-MD, Born–Oppenheimer density functional theory; TDDFT, time-dependent DFT; QBE, quantum Boltzmann equation; and NEGF, Nonequilibrium Green functions. Figure modified from Phys. Plasmas 27, 042710 (2020)

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