P 14: Codes and modelling

Time: Wednesday 14:00–15:55 Location: b302

P 14.1 Wed 14:00 b302

Quantum hydrodynamics for plasmas – quo vadis? — •Michael Bonitz[1], Zhandos Moldabekov[2], Hanno Kählert[1], and Shen Zhang[1] — [1]Institut für Theoretische Physik und Astrophysik, Universität Kiel, Leibnizstr. 15 — [2]Al Farabi University, Almaty, Kazakhstan

Quantum hydrodynamics (QHD) has become popular for modeling quantum plasmas and warm dense matter, following Ref. 1. While QHD is quite successful for describing Bose-Einstein condensates and plasmonic excitations in metallic nanoparticles, the application of the model of Ref. [1] to dense plasmas has lead to oversimplified fluid equations. These equations neither reproduce the correct plasmon dispersion (except for 1D models) nor the screened potential of an ion in a quantum degenerate plasma [2, 3] and have led to astonishing predictions that have been controversially discussed. Here we present a systematic derivation, starting from quantum statistical theory, that leads to microscopic QHD equations that are in agreement with time-dependent DFT and quantum kinetic theory and which serve as a basis for deriving improved QHD models for plasmas [3].

[1] G. Manfredi and F. Haas, Phys. Rev. B **74**, 075316 (2001)
[2] Zh. Moldabekov, M. Bonitz, and T. Ramazanov, Phys. Plasmas **25**, 031903 (2018)
[3] M. Bonitz, Zh. Moldabekov, and T. Ramazanov, Phys. Plasmas **26**, 090601 (2019)

P 14.2 Wed 14:25 b302

Ionization in high-density plasmas: an ab initio study for carbon at Gbar pressures — Mandy Bethkenhagen[1], Bastian B. L. Witte[1,2], Gerd Röpke[1], Tilo Döppner[3], Dominik Kraus[4,5], Siegfried H. Glenzer[2], and •Ronald Redmer[1] — [1]Institut für Physik, Universität Rostock, 18051 Rostock — [2]SLAC National Accelerator Laboratory, 2575 Sand Hill Road, Menlo Park, CA 94025 USA — [3]LLNL, Livermore, CA 94550, USA — [4]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden — [5]Institute of Solid State and Materials Physics, TU Dresden, 01069 Dresden

We apply density functional theory molecular dynamics (DFT-MD) simulations to calculate the ionization degree of plasmas in the warm dense matter regime. Standard descriptions of the ionization potential depression (IPD) have been challenged recently by experiments approaching unprecedentedly high densities indicating that improved IPD models are required to describe warm dense matter. We propose a novel ab initio method to calculate the ionization degree directly from the dynamic electrical conductivity using an exact sum rule. This approach is demonstrated for carbon at a temperature of 100 eV and pressures in the Gbar range. We find substantial deviations from widely applied IPD models like Stewart-Pyatt and Ecker-Kröll implying that condensed matter and quantum effects like band structure and Pauli blocking need to be included explicitly in ionization models. Our results will help to precisely model matter under conditions occurring, e.g., during inertial confined fusion implosions or inside astrophysical objects such as brown dwarfs and low-mass stars.

P 14.3 Wed 14:40 b302

***Ab initio* simulation results for the dynamic properties of warm dense matter** — •Michael Bonitz[1], Paul Hamann[1], Tobias Dornheim[2], and Alexey Filinov[1] — [1]Institut für Theoretische Physik und Astrophysik, Universität Kiel, Leibnizstr. 15 — [2]Center for Advanced Systems Understanding (CASUS), Görlitz, Germany

Warm dense matter (WDM) – an exotic state where electrons are quantum degenerate and ions may be strongly correlated – is ubiquitous in astrophysics and highly compressed laboratory plasmas. We have recently obtained *ab initio* thermodynamic results for the electron component in WDM based on novel quantum Monte Carlo (QMC) simulations [1, 2] including the first *ab initio* parametrization of the exchange-correlation free energy F_xc [2, 3]. Moreover, recently the first exact QMC results for the dynamic local field correction and the dynamic structure factor could be obtained [4]. An interesting result is the prediction of a negative plasmon dispersion – an effect that should be observable in dense hydrogen.

[1] T. Dornheim, S. Groth, T. Sjostrom, F.D. Malone, W.M.C. Foulkes, and M. Bonitz, Phys. Rev. Lett. **117**, 156403 (2016)
[2] S. Groth, T. Dornheim, T. Sjostrom, F.D. Malone, W.M.C. Foulkes, and M. Bonitz, Phys. Rev. Lett. **119**, 135001 (2017)
[3] T. Dornheim, S. Groth, and M. Bonitz, Phys. Reports **744**, 1-86 (2018)
[4] T. Dornheim, S. Groth, J. Vorberger, and M. Bonitz, Phys. Rev. Lett. **121**, 255001 (2018)

P 14.4 Wed 14:55 b302

Molecular dynamics study of non-equilibrium dense plasmas with ionization potential depression — •Rui Jin[1,2], Malik Muhammad Abdullah[1,3,4], Zoltan Jurek[1,3], Sang-Kil Son[1,3], and Robin Santra[1,3,4] — [1]Center for Free-Electron Laser Science, DESY, Hamburg, Germany — [2]Department of Physics and Astronomy, Shanghai Jiaotong University, Shanghai, China — [3]The Hamburg Centre for Ultrafast Imaging, Hamburg, Germany — [4]Department of Physics, Universität Hamburg, Hamburg, Germany

High energy density matter exists extensively in the universe, from hot dense plasmas such as supernova and stellar interiors to warm dense matter such as planetary interiors. Creating and analyzing hot and warm dense plasmas under such extreme conditions in the laboratory is critical to understand their unique properties. The advent of x-ray free-electron laser (XFEL), which provides intense femtosecond pulses, enables us to quickly heat bulk materials, creating dense plasmas under non-local thermal equilibrium (NLTE). In the dense plasma, ionization potential depression (IPD) effect emergies, but theoretical IPD models have been considered at local thermal equilibrium. In this study, we employ XMDYN, a Monte-Carlo (MC) and molecular-dynamic (MD) -based computational tool, to simulate the dense materials interacting with intense XFEL pulses. In order to include the IPD for NLTE plasma environment, we propose a numerical method based on ab initio calculation of atomic energy shifts due to the micro-field obtained directly from MD simulations. We demonstrate the the IPD effects in MD simulations of solid-density aluminum plasma formation.

P 14.5 Wed 15:10 b302

PICLS: a gyrokinetic full-f particle-in-cell code for open field line simulations — •Mathias Boesl, Andreas Bergmann, Alberto Bottino, David Coster, and Frank Jenko — Max Planck Institut für Plasmaphysik, D-85748 Garching, Germany

While in recent years, gyrokinetic simulations have become the workhorse for theoretical turbulence and transport studies in the plasma core, their application to the edge and scrape-off layer (SOL) region presents significant challenges. The "full-f" code PICLS has been developed, to in particular study the SOL region with its steep density and temperature gradients as well as large fluctuation amplitudes. PICLS is based on an electrostatic full-f model with a linearized field equation and uses kinetic electrons. The electrostatic potential is calculated via the polarization equation, with the help of B-spline finite-elements for the charge deposition and the field solver. In this talk, we will introduce the PICLS model and show our results of applying it to the well-studied 1D parallel transport problem during an edge-localized mode (ELM) for the non-collisional and collisional case. Our current progress on extending PICLS towards three spatial domains, will be presented and key features for the 3D extension, such as field solver and particle pusher, will be shown.

P 14.6 Wed 15:25 b302

Particle in Cell Simulations for the KATRIN Experiment — •Jonas Kellerer, Christian Reiling, and KATRIN Collaboration — Karlsruhe Institute of Technology (KIT), ETP, Postfach 3640, 76021 Karlsruhe

The **Kar**lsruhe **Tri**tium **N**eutrino (KATRIN) experiment aims to determine the effective neutrino mass through spectroscopy of gaseous Tritium β-decay. Those high energy β-decay electrons ionize the surrounding gas in the source and thus create a partly ionized plasma. The exterior experimental conditions generate unconventional plasma conditions resulting in an highly magnetized, partly collisional, multi-species, non-thermal (with thermal components), bound plasma. The combination of these properties make an analytical description impossible. Thus we decided on a two folded iterative simulation approach: the slow ion physics will be covered by the newly developed Monte Carlo code KARL, which produces electron energy distributions and

ion currents. These results will be used by the well tested ACRONYM Particle in Cell code to resolve the fast electron-field interactions. The derived fields are in turn used as input for the KARL code. To accommodate for the special experimental conditions we implemented curve-shaped boundaries in the conformal FDTD algorithm, following the Dey-Mittra algorithm. Hereby we took extra care on the electron-wall interactions. Supplementary we added electromagnetic background fields mimicking the use external power supplies.

P 14.7 Wed 15:40 b302

Dynamic structure factor of Yukawa liquids: molecular dynamics simulations and memory function approach — •Hanno Kählert — ITAP, Christian-Albrechts-Universität zu Kiel

Molecular dynamics simulations are used to compute the dynamic structure factor (DSF) of a strongly coupled Yukawa liquid over a wide range of coupling strengths. Despite its simplicity, the Yukawa model is of relevance for a variety of systems, including dense plasmas or strongly coupled dusty plasmas. The results for the DSF are compared with a theoretical approach based on the memory function formalism. In particular, a memory function incorporating viscoelastic effects [1] is applied to model the collective behavior of the Yukawa liquid at long wavelengths and low frequencies. Fitting the model to the simulation data allows one to estimate transport coefficients such as the viscosity. In addition, the fluctuation-dissipation theorem and the Kramers-Kronig relations are used to compute the complex density response function, which makes it possible to obtain the memory function directly from the simulation data.

[1] U. Bafile, E. Guarini, and F. Barocchi, Phys. Rev. E **73**, 061203 (2006).