# P 12: Theory and Modelling I

Zeit: Dienstag 16:30–18:30 Raum: HS Foyer

P 12.1 Di 16:30 HS Foyer

**Ab Initio Quantum Monte Carlo Simulation of the Warm Dense Electron Gas** — Tobias Dornheim[1], Simon Groth[1], •Travis Sjostrom[2], and Michael Bonitz[1] — [1]Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — [2]Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA

The uniform electron gas (UEG) at finite temperature is of high interest for warm dense matter research, most notably as an input for thermal density functional theory. Until recently, the most accurate data [1] had been obtained using Quantum Monte Carlo (QMC) in the fixed node approximation (RPIMC) and by subsequently extrapolating the results for the finite model system to the thermodynamic limit (TDL) by adding a finite-size correction. However, the quality of these results has been called into question: (I) RPIMC constitutes an uncontrolled approximation that induced errors of $\sim 10\%$ for the finite model system [2] and (II) the employed finite-size correction is only appropriate in parts of the warm dense regime. Here we show how to perform ab initio QMC simulations of the UEG without the fixed node approximation [3] and present a new approach to subsequently extrapolate the results to the TDL without any systematic errors [4].
[1] E. Brown et al., PRL **110**, 146405 (2013)
[2] T. Schoof et al., PRL **115**, 130402 (2015)
[3] T. Dornheim et al., PRB **93**, 205134 (2016)
[4] T. Dornheim et al., PRL **117**, 156403 (2016)
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P 12.2 Di 16:30 HS Foyer

**Theoretical foundations of quantum hydrodynamics for dense plasmas** — •Zhandos Moldabekov and Michael Bonitz — Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel, Leibnizstraße 15, 24098 Kiel, Germany

Dense quantum plasmas are of high current interest in astrophysics and many laboratory experiments. The theory of these systems is complicated, therefore a simplified approach based on Quantum hydrodynamics (QHD) has become popular [1]. However, often QHD is used outside the range of applicability and even with incorrect explicit expressions. The key ingredients of QHD for fermions are the Fermi pressure and the Bohm potential. We have recently shown [2] that to compute the screened potential in a plasma the prefactor of the Bohm term has to be corrected yielding good agreement with the static long-wavelength limit of the random phase approximation [3]. Here we analyze how the QHD equations can be further improved in order to better reproduce a broader wavenumber-frequency range. The nonlocal Bohm potential, in linear response, has been derived. The exchange-correlation potential in linear response, in terms of the dynamic local field correction, for the QHD application has been obtain. This allows to use the results of the previous studies of the dynamic local field correction in the QHD theory.

[1] G. Manfredi, F. Haas, Phys. Rev. B 64, 075316 (2001) [2] D. Michta et al., Contrib. Plasma Phys. 55, 437 (2015) [3] Z. Moldabekov et al., Phys. Plasmas 22, 102104 ((2015)

P 12.3 Di 16:30 HS Foyer

**Diagnostik und Modellierung eines Mikrowellen-Plasmabrenners bei Atmosphärendruck** — •Sandra Gaiser[1], Andreas Schulz[1], Matthias Walker[1] und Thomas Hirth[2] — [1]Institut für Grenzflächenverfahrenstechnik und Plasmatechnologie, Universität Stuttgart — [2]Karlsruher Institut für Technologie

Für die Untersuchung und Optimierung eines bei Atmosphärendruck betriebenen Mikrowellen-Plasmabrenners wurden mit Hilfe des Programmes COMSOL Multiphysics® Simulationsmodelle erstellt. Die Ergebnisse der Simulationen konnten mit experimentellen Daten verglichen werden.

Das Plasmamodell enthält Bilanzgleichungen für die Elektronen- und Schwerteilchendichten sowie für die Elektronenenergie. Dazu kommt ein Satz von Elementarreaktionen zur Beschreibung eines Argon-Plasmas. Des Weiteren wurde das Drude-Modell verwendet, um dem Plasma eine frequenzabhängige Leitfähigkeit und Permittivität zuzuweisen und damit seine elektrischen Eigenschaften zu berücksichtigen. Dies ermöglicht es, die Auswirkung einer sich ändernden Elektronendichteverteilung auf das elektrische Feld im Plasmabrenner zu untersuchen.

Ein Vergleich der berechneten maximalen Elektronendichte mit gemessenen Werten zeigte bereits eine gute Übereinstimmung von Simulation und Experiment. Qualitative Untersuchungen des Plasmas bestätigten zudem einen aus den Simulationsergebnissen abgeleiteten Zusammenhang zwischen der Lage des Plasmas im Brenner und einer einhüllenden Gasströmung.

P 12.4 Di 16:30 HS Foyer

**Effect of mode structure variation on fast particle transport in hybrid-kinetic simulations** — •Thomas Hayward-Schneider and Philipp Lauber — Max-Planck-Institut für Plasmaphysik, Garching, Germany

Perturbative modelling of Alfvén eigenmodes (AEs) using the nonlinear perturbative drift-kinetic initial value code Hagis and the linear gyrokinetic eigenvalue code Ligka is introduced. We present the steps to couple these two codes, with a goal of non-/semi- perturbative, nonlinear simulations of AEs. Towards this aim, we show a benchmark of a prescribed, time-dependent mode structure in Hagis. We introduce ITER scenarios for study, and observe that the AE resonance locations are highly sensitive to the magnetic profiles.

P 12.5 Di 16:30 HS Foyer

**Molecular Dynamics Simulations Of Laser Ablation and Plasma Formation** — Eugen Eisfeld and •Johannes Roth — Universität Stuttgart

Laser ablation is studied with classical molecular dynamics simulations. The interaction of ultrashort laser pulses with a metallic material is modeled using a hybdrid two-temperature model with separate temperatures for the electrons and the lattice. We have implemented an ionization model based on the Thomas-Fermi theory as well as wide-range models for the complex permittivity, the electronic heat conductivity and the electron-phonon coupling parameter, similar to the work of Povarnitsyn [1] which describes the transition from the metal to the plasma state.

The laser absorption is calculated by solving the Helmholtz wave equation instead of the simple Lambert-Beer law. The improved results are compared to simulations carried out with hydrodynamic simulations.

[1] Povarnitsyn et al., Appl. Surf. Sci. 258 (2012) 9480.