HOSTED BY

HELMHOLTZ ZENTRUM
DRESDEN ROSSENDORF

CASUS
CENTER FOR ADVANCED
SYSTEMS UNDERSTANDING

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WELCOME

We welcome you to the Strongly Coupled Coulomb Systems Conference 2022 in Görlitz hosted by the Center for Advanced Systems Understanding at the Helmholtz-Zentrum Dresden-Rossendorf.

The SCCS Conference Series brings together scientists working on the diverse aspects of many-body systems that are characterized by the single unifying theme of strong Coulomb long-range interactions. The Series focuses on common behaviors of such systems and on common techniques for dealing with them across disciplines.

It is our great pleasure to host this edition of the SCCS Conference Series primarily in person, thereby providing an international venue for the exchange of scientific ideas in an open, friendly, and inclusive environment. The ongoing COVID-19 pandemic has posed great challenges to our global society. We take these seriously and strive to ensure a safe venue by following the current guidelines on preventive measures.

Following the long-standing tradition of SCCS, the Program Committee has put together a compelling scientific program connecting the astrophysics, plasma physics, and condensed-matter physics communities from around the world. This edition of the Conference Series will cover scientific sessions on Dense and Astrophysical Plasmas, Plasmas in Condensed Matter, Confined and Mesoscopic Coulomb Systems, High-Energy Density Plasmas in the Laboratory, Classical Charged Systems, and Developments in Theoretical Methods and Numerical Techniques. In addition, the emerging topic of artificial intelligence will be highlighted this year in terms of a special session on machine-learning methods for Coulombic systems. This is an active research area of the newly founded host institute in Görlitz that focuses on digital systems research.

We look forward to a week packed with excellent science and stimulating discussions!

Attila Cangi
Tobias Dornheim
Local Organizing Committee SCCS 2022

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Conference History

NATO Advanced Study Institute on Strongly Coupled Plasmas
1977 Orleans-la-Source, France (Feix, Kalman and Carini)

Les Houches Winter School
1982 Les Houches, France (Baus and Hansen)

Strongly Coupled Plasmas
1986 Santa Cruz, California, USA (Rogers and DeWitt)
1989 Lake Yamanaka, Japan (Ichimaru)
1992 Rochester, New York, USA (Van Horn and Ichimaru)
1995 Binz, Germany (Kraeft and Schlanges)

Strongly Coupled Coulomb Systems
1997 Boston, Massachusetts, USA (Kalman)
1999 St. Malo, France (Deutsch and Jancovici)
2002 Santa Fe, USA (Murillo and Benage)
2005 Moscow, Russia (Fortov and Norman)
2008 Camerino, Italy (Neilson and Senatore)
2011 Budapest, Hungary (Donko and Hartmann)
2014 Santa Fe, USA (Graziani)
2017 Kiel, Germany (Bonitz, Ludwig and Moldabekov)
2022 Görlitz, Germany (Cangi and Dornheim)

GENERAL REMARKS

Conference website:
https://events.hifis.net/e/SCCS2022

WIFI
ssid: **Synagoge** | pw: **KulturGR**

Points of contact (from 9 am to 8 pm)

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SUNDAY, July 24

15^{00} - 18^{00} Registration

MONDAY, July 25

8^{30} - 8^{40} Introduction by LOC Chair

8^{40} - 9^{00} Welcome by HZDR Director

9^{00} - 10^{45} **Dense and Astrophysical Plasmas: 1**

9^{00} ***Ab Initio Simulations for Warm Dense Matter with Applications in Planetary Physics***
Speaker: Burkhard Militzer (University of California, Berkeley, United States)

9^{50} ***Density Functional Theory calculations for high- temperature carbon plasmas***
Speaker: Mandy Bethkenhagen (ENS Lyon, France)

10^{25} ***Electronic transport coefficients of hydrogen from density functional theory across the plasma plane***
Speaker: Martin French (Institute of Physics, University of Rostock, Rostock, Germany)

10^{45} - 11^{15} Coffee Break

11^{15} - 12^{30} **Dense and Astrophysical Plasmas: 2**

11^{15} ***Mean Force Kinetic Theory***
Speaker: Scott Baalrud (University of Michigan, United States)

11^{50} ***Dynamical formation of the Diamond rain in icy giant planets by C-H immiscibility***
Speaker: Bo Chen (National University of Defense Technology, China)

12^{10} ***Electrical Conductivity of Iron in Earth's Core from Microscopic Ohm's Law***
Speaker: Kushal Ramakrishna (CASUS, Helmholtz-Zentrum Dresden-Rossendorf, Germany)

12^{30} - 14^{30} Lunch Break

14^{30} - 16^{15} **High-Energy Density Plasmas in the Laboratory: 1**

14^{30} ***Pressure effects on the electronic structure of carbon-hydrogen mixtures in the Mbar to Gbar regime***
Speaker: Dominik Kraus (University of Rostock, Germany)

SCHEDULE

15^{20} ***Spectral line shapes in dense plasmas***
Speaker: Evgeny Stambulchik (Weizmann Institute of Science, Israel)

15^{55} ***Sensitivity of uniaxially driven ICF target performance to interfacial conduction in the high-energy-density regime***
Speaker: Dave Chapman (First Light Fusion Ltd, Oxford, United Kingdom)

16^{15} - 16^{45} Coffee Break

16^{45} - 18^{00} **High-Energy Density Plasmas in the Laboratory: 2**

16^{45} ***Direct imaging of phase transitions in nonequilibrium warm dense matter***
Speaker: Mianzhen Mo (SLAC National Accelerator Laboratory, United States)

17^{20} ***Ion core effect on transport and thermodynamic properties in dense plasmas***
Speaker: Tlekkabul Ramazanov (Al Farabi Kazakh National University, IETP, Kazakhstan)

17^{40} ***Accurate and efficient calculations of mean ionization states with an average-atom model***
Speaker: Timothy Callow (CASUS, Helmholtz-Zentrum Dresden-Rossendorf, Germany)

18^{00} - 20^{00} Poster Session

TUESDAY, July 26

9^{00} - 10^{45} **Confined and Mesoscopic Coulomb Systems: 1**

9^{00} ***Coulomb effects in electronic transport***
Speaker: Narozhny Boris (KIT, Germany)

9^{50} ***Itinerant-electron magnetism: the importance of many-body correlations***
Speaker: Saverio Moroni (IOM CNR and SISSA, Trieste, Italy)

10^{25} ***Transport evidence for a sliding two-dimensional quantum electron solid***
Speaker: Sergey Kravchenko (Northeastern University, United States)

10^{45} - 11^{15} Coffee Break

11^{15} - 12^{30} Confined and Mesoscopic Coulomb Systems: 2

11^{15} ***Excitonic condensation, pairing gap and quadriexcitons in an electron-hole bilayer with twofold valley degeneracy***
Speaker: Stefania De Palo (IOM-CNR, Italy)

11^{50} ***Supersolid state of a dilute exciton gas in electron-hole bilayers***
Speaker: Dmytro Fil (Institute for Single Crystals of National Academy of Sciences of Ukraine, Ukraine)

12^{10} ***Exciton supersolid phase transition in bilayer semiconductors***
Speaker: Sara Conti (University of Antwerp, Belgium)

12^{30} - 14^{30} Lunch Break

14^{30} - 15^{30} Dense and Astrophysical Plasmas: 3

14^{30} ***Carbon ionization in the hot dense regime***
Speaker: Jean Clerouin (CEA/DAM/DIF, Arpajon, France)

14^{50} ***Dynamic Structure Factor of the Magnetized One-Component Plasma: Crossover from Weak to Strong Coupling***
Speaker: Hanno Kählert (ITAP, Kiel University, Germany)

15^{10} ***Ab initio simulations for the ion-ion structure factor of warm dense aluminum***
Speaker: Maximilian Schörner (Universität Rostock, Germany)

15^{30} - 16^{30} High-Energy Density Plasmas in the Laboratory: 3

15^{30} ***Electronic pair alignment and roton feature in the warm dense electron gas***
Speaker: Tobias Dornheim (CASUS, Helmholtz-Zentrum Dresden-Rossendorf, Germany)

15^{50} ***Waves in the medium and on the boundary of Quark-Gluon Plasma***
Speaker: Kassymkhan Baiseitov (Al-Farabi Kazakh National University, Kazakhstan)

16^{10} ***Electron–atom interaction in dense plasma of noble gases***
Speaker: Karlygash Dzhumagulova (IETP, al-Farabi Kazakh National University, Kazakhstan)

16^{30} - 17^{00} Coffee Break

SCHEDULE

17^{00} - 18^{00} Confined and Mesoscopic Coulomb Systems: 3

17^{00} ***Interaction induced topological collective edge excitations in layered structures***
Speaker: Abedinpour Harzand Saeed (Institute for Advanced Studies in Basic Sciences (IASBS), Iran)

17^{20} ***High-Tc electron-hole superfluidity and BCS-BEC crossover in double-layer heterostructures***
Speaker: Andrea Perali (School of Pharmacy, Physics Unit, University of Camerino, Italy)

17^{40} ***Anomalous Josephson effect in chiral double layers***
Speaker: Klaus Ziegler (Institute of Physics, University Augsburg, Germany)

WEDNESDAY, July 27

9^{00} - 10^{45} Plasmas in Condensed Matter: 1

9^{00} ***Collective modes in beyond-graphene atomically thin materials***
Speaker: Marco Polini (University of Pisa, Italy)

9^{50} ***Eliashberg theory of superconductivity from electronic collective excitations***
Speaker: Saverio Moroni (IOM CNR and SISSA, Trieste, Italy)

10^{25} ***Ultrafast dynamics of quantum many-body systems including dynamical screening and strong coupling***
Speaker: Michael Bonitz (ITAP, Kiel University, Germany)

10^{45} - 11^{15} Coffee Break

11^{15} - 12^{30} Plasmas in Condensed Matter: 2

11^{15} ***Quantum geometric plasmonics: Berry curvature, quantum metric, and spontaneous collective mode ferromagnetism***
Speaker: Justin Song (Nanyang Technological University, Singapore)

11^{50} ***Collective excitations and quantum incompressibility in electron-hole fluids***
Speaker: Gaetano Senatore (Dipartimento di Fisica, Università degli studi di Trieste, Italy)

12^{10} ***Debye plasma model under scrutiny: Rydberg excitons as testing probes for low-density electron-hole plasmas***
Speaker: Dirk Semkat (Institut für Physik, Ernst-Moritz-Arndt-Universität Greifswald, Germany)

12^{30} - 14^{30} Lunch Break

14^{30} - 16^{00} Free Discussion Time

16^{00} - 18^{00} Guided City Tours

19^{00} - 22^{00} Conference Dinner

THURSDAY, July 28

9^{00} - 10^{45} Classical Charged Systems: 1

9^{00} ***Fast Simulations of Complex Charged Systems for Soft Matter Applications***
Speaker: Christian Holm (Institut für Computerphysik, Universität Stuttgart, Germany)

9^{50} ***Investigation of the fluctuation-theorem convergence in a dusty plasma experiment***
Speaker: Yan Feng (Soochow University, China)

10^{25} ***Algebraic infection of charge correlations of a classical electrolyte at the critical point of the liquid-gas transition***
Speaker: Angel Alastuey (Laboratoire de Physique, ENS de Lyon and CNRS, France)

10^{45} - 11^{15} Coffee Break

11^{15} - 12^{30} Classical Charged Systems: 2

11^{15} ***Emergent Coulomb Fluids in Spin Ice***
Speaker: Peter Holdsworth (ENS Lyon, France)

11^{50} ***Strong Correlation Effects in Atmospheric Pressure Plasmas***
Speaker: Marco Acciarri (NERS, University of Michigan, United States)

12^{10} ***Charing of dust particles in space***
Speaker: Ranna Masheyeva (IETP, Al-Farabi Kazakh National University, Almaty, Kazakhstan)

12^{30} - 14^{30} Lunch Break

14^{30} - 15^{30} Plasmas in Condensed Matter: 3

14^{30} ***Ultradilute quantum liquid of dipolar atoms in a bilayer***
Speaker: Jordi Boronat (Universitat Politecnica de Catalunya, Spain)

14^{50} ***Microfluidic flow in single-layer dusty plasmas***
Speaker: Peter Hartmann (Wigner Research Centre for Physics, Hungary)

15^{10} ***Coulomb gas sum rules for vortex-pair fluctuations in 2D superfluids***
Speaker: Gary Williams (University of California, Los Angeles, United States)

15^{30} - 16^{30} Classical Charged Systems: 3

15^{30} ***Phase separation/diagram of dusty plasmas***
Speaker: Hiroo Totsuji (Okayama University, Japan)

SCHEDULE

15^{50} ***Dynamics of defect filaments in weakly disordered dust acoustic waves of dusty plasmas***
Speaker: Lo Wei-Shuo (Department of Physics, National Central University, Taiwan)

16^{10} ***The Conductivity of Concentrated Electrolytes***
Speaker: Yael Avni (Tel Aviv University, Israel)

16^{30} - 17^{00} Coffee Break

17^{00} - 18^{00} Developments in Theoretical Methods and Numerical Techniques: 1

17^{00} ***Classical Coulomb bridge functions in classical and quantum plasma liquids***
Speaker: Tolias Panagiotis (Space and Plasma Physics—KTH Royal Institute of Technology, Sweden)

17^{20} ***Development of a new Quantum Trajectory Molecular Dynamics Framework***
Speaker: Pontus Svensson (University of Oxford, United Kingdom)

17^{40} ***Speeding up X-ray-matter molecular dynamics simulation tool XMDYN with tree algorithms***
Speaker: Michal Stransky (European XFEL, Germany)

FRIDAY, July 29

9^{00} - 10^{45} Developments in Theoretical Methods and Numerical Techniques: 2

9^{00} ***The dynamic nature of high-pressure ice VII and a theory for dynamic phases behind it***
Speaker: Xin-Zheng Li (Peking University, China)

9^{50} ***Stochastic Vector Techniques for Strongly Coupled Coulomb Systems***
Speaker: Roi Baer (The Hebrew University, Israel)

10^{25} ***Electronic stopping in warm dense matter using Ehrenfest dynamics and time-dependent density functional theory***
Speaker: Alina Kononov (Sandia National Laboratories, United States)

10^{45} - 11^{15} Coffee Break

11^{15} - 12^{30} Developments in Theoretical Methods and Numerical Techniques: 2

11^{15} ***Like-charge attraction in one- and two-dimensional Coulomb systems***
Speaker: Gabriel Tellez (Universidad de los Andes, Colombia)

11^{50} ***Thermodynamic and transport properties of plasmas: numerical simulations and benchmarks from analytical theory***
Speaker: Gerd Röpke (Institute of Physics, University of Rostock, Germany)

12^{10} ***Analyzing XC functionals for electronic structure calculations at WDM parameters***
Speaker: Zhandos Moldabekov (CASUS, Helmholtz-Zentrum Dresden-Rossendorf, Germany)

12^{30} - 14^{30} Lunch Break

14^{30} - 15^{45} Machine-Learning Methods for Coulomb Systems: 1

14^{30} ***Deep Quantum Monte Carlo***
Speaker: Frank Noe (FU Berlin, Germany)

15^{05} ***Stochastic Representation of Many-Body Quantum States***
Speaker: Guy Cohen (Tel Aviv University, Israel)

15^{25} ***Towards Large-Scale and Spatio-temporally Resolved Diagnosis of Electronic Density of States by Deep Learning***
Speaker: Qiyu Zeng (National University of Defense Technology, China)

15^{45} - 16^{15} Coffee Break

16^{15} - 17^{10} Machine-Learning Methods for Coulomb Systems: 2

16^{15} ***FermiFlow: a variational free-energy approach for fermions in the continuum***
Speaker: Lei Wang (Chinese Academy of Sciences, Beijing, China)

16^{50} ***Data-Driven and Physics-Informed Modeling of Matter under Extreme Conditions***
Speaker: Attila Cangi (CASUS, Helmholtz-Zentrum Dresden-Rossendorf, Germany)

17^{10} - 17^{30} Closing Remarks

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ABSTRACTS

“Interaction induced” topological collective edge excitations in layered structures

Saeed H. Abedinpour*[1], Fatemeh Pouresmaeeli[1], Maryam Darivishi[3]

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We study the collective density oscillations of layered structures. We illustrate how for interacting bosons, the resonance condition for the density oscillations in the linear response regime could be expressed as a general eigenvalue problem. This suggests that a non-zero Berry phase could be obtained with a suitable tuning of the system parameters in an alternating layered structure [see, Fig. 1]. The topologically non-trivial phase of such a system supports topological collective excitations localized at the edges of the system. In particular, the condition for having topological excitations depends on the wave vector of the excitation, and therefore it is possible to have localized excitations only for some ranges of the wavelengths. We then try to carry on the same idea for interacting fermions and discuss how it is possible to engineer topological edge plasmons in layered materials.

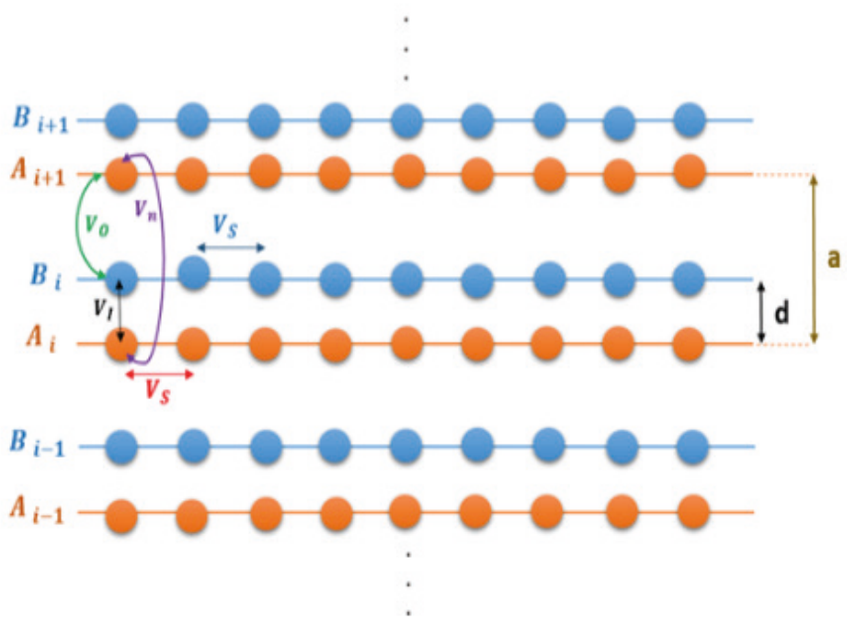

Figure 1: Illustration of a layered structure with two different types of layers.

[1] F. Pouresmaeeli, M. Darvishi, and S. H. Abedinpour, in preparation.

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Strong Correlation Effects in Atmospheric Pressure Plasmas

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1 NERS, University of Michigan, Ann Arbor, United States of America | 2 Sandia National Laboratories, Albuquerque, New Mexico, United States of America

In this work, a partially ionized atmospheric pressure plasma was simulated using Molecular Dynamics (MD) at different ionization fractions from a random distribution of neutral particles, after a short and uniform ionization pulse was applied. Short (neutral-neutral), medium (charge-neutral) and long (charge-charge) range interactions were included while considering the electrons as a background non-interacting species. Ion and neutral temperature evolution, diffusion coefficients and radial distribution functions were computed in order to study the transport properties of the plasma and the correlation of the different interactions involved. Disorder Induced Heating (DIH) was observed at the beginning of the discharge for all the ionization fractions simulated, followed by fluctuations due to energy exchange between ion kinetic energy and Coulomb potential energy as a result of the high coupling strength of ion-ion interactions. After the DIH, ion temperature relaxation was observed due to collisions between ion and neutral species. The ion temperature relaxation time was calculated and agreed with the molecular dynamics simulation results. An additional heating was observed due to the ion-neutral three body recombination at a much longer time scale compared to the ion temperature relaxation time. The equilibrium temperature and ion-ion Coulomb coupling strength computed from the theory agreed with the results obtained from the MD simulations. The observed effects suggest that atmospheric pressure plasmas are sufficiently dense that they are influenced by strong correlation effects associated with many-body interactions that are not treated in the dilute limit.

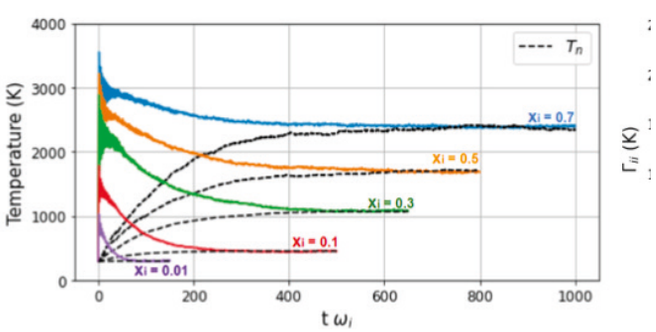

Figure 1: Ion and Neutral gas temperature evolution during the MD simulation for different ionization fraction xi.

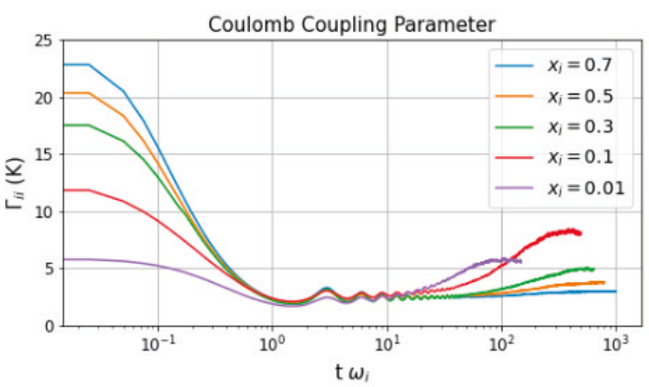

Figure 2: Evolution of the Coulomb coupling parameter during the discharge for different xi.

This work is supported by DOE FES grant No. DE-SC0022201, and the LDRD program at Sandia National Laboratories under contract DE-NA-0003525.

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Algebraic infection of charge correlations of a classical electrolyte at the critical point of the liquid-gas transition

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We consider a classical Two-Component Plasma analog of the Restricted Primitive Model for an electrolyte, where the hard-core interaction is replaced by a soft differentiable potential. Within the Born-Green-Yvon hierarchy for the equilibrium distribution functions, we shed light on an infection mechanism where the charge correlations are polluted by the density correlations at the critical point of the liquid-gas transition. This implies an algebraic decay of critical charge correlations. Such breakdown of exponential clustering should provide dielectric rather than conducting properties at the critical point, leading to the violation of certain charge-charge sum rules. This is in agreement with Monte Carlo simulations.

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Time resolved opacity maps of warm dense Ti: a Bayesian search of coupling parameters

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Dense, strongly coupled plasmas are challenging to model due to the difficulty of treating the quantum many-body interactions at elevated temperatures. Electron-electron (e-e) and electron-ion (e-i) collisions determine the basic plasma properties, yet are difficult to calculate. Moreover, isolating and measuring the different scattering rates in thermal equilibrium is impossible. Here, we describe a femtosecond pump-probe experiment that drives a solid into the plasma state to measure the e-e and e-i couplings.

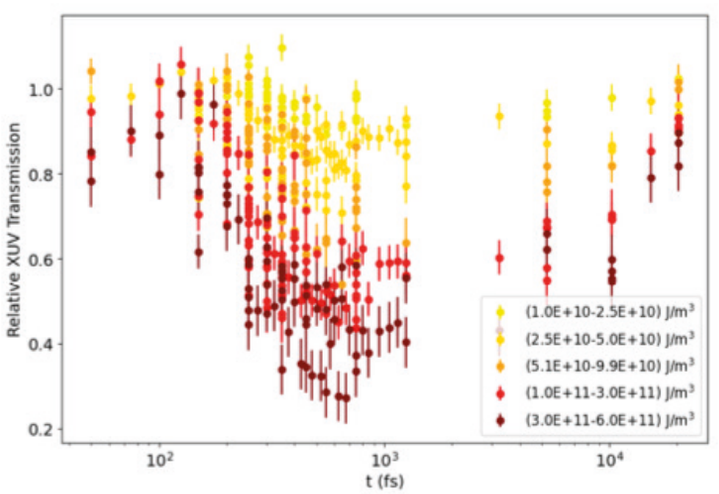

Figure 1: Relative to cold XUV transmission, as a function of time. Laser peaks at 250 fs

An experimental set up consisting of an ultrashort infra-red laser pulse (1014 W/cm2, 50 fs, 800 nm) was used to create up to tens of eV solid-density plasma in the skin depth of a Ti metal film. The electronic structure of the heated sample was probed by sending a XUV pulse with energy close to that of the M2,3 absorption edge. The transmitted XUVs spatial profile was recorded in a single-shot with 10 µm resolution, and scanned with up to 50 fs resolution, for tens of picoseconds. A map of XUV transmission for variable laser fluences was then recorded in every shot. The results are shown in figure 1, where a first electronic excitation from the laser gives way (in the ps regime) to e-i equilibration with subsequent cooling of the electrons and recovery of the transmission.

To interpret the experimental data concerning the first picosecond, a model was constructed using quantum kinetic calculations, inspired by [1]. A screened Coulomb potential and uniform heating through the depth of the material were considered and a nearly free electron gas interacting with fixed scattering centres and other gas particles was assumed. For the longer time response, a two temperatures model was used where the e-i coupling parameter was calculated as in [2].

Finally, a MCMC search was performed so as to estimate the posterior distribution of the free parameters. This approach allows to properly account for the multiple leading order contributions, their correlations, and a better understanding of the parameter space.

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The Conductivity of Concentrated Electrolytes

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The conductivity of ionic solutions is arguably their most important trait, being widely used in electrochemical, biochemical, and environmental applications. The Debye- Hückel-Onsager theory successfully predicts the conductivity at very low ionic concentrations of up to a few millimolars, but there is no well-established theory applicable at higher concentrations. We study the conductivity of ionic solutions using a stochastic density functional theory, paired with a modified Coulomb interaction that accounts for the hard-core repulsion between the ions. The modified potential suppresses unphysical, short-range electrostatic interactions, which are present in the Debye-Hückel-Onsager theory. Our results for the conductivity show very good agreement with experimental data up to 3 molars, without any fit parameters (see Fig. 1). We provide a compact expression for the conductivity, accompanied by a simple analytical approximation.

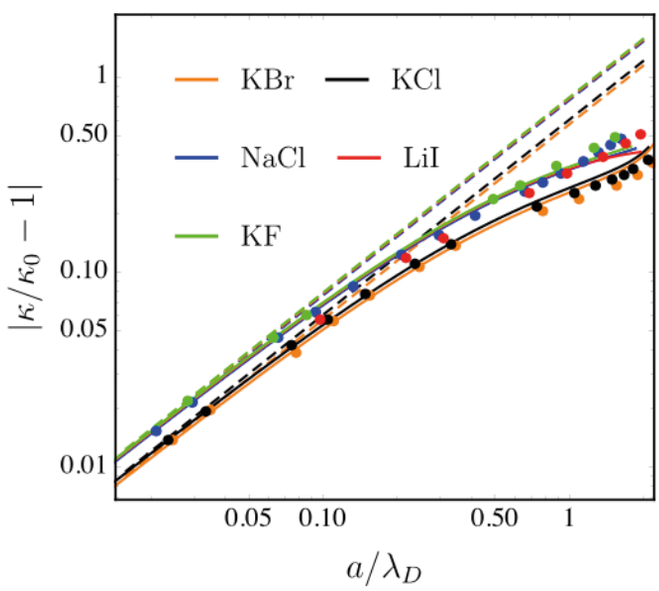

Figure 1: The relative conductivity correction as a function of the distance of closest approach divided by the screening length, for different salts on a log-log plot. Dots - experimental data; Full lines - numerical result; Dashed lines - the DHO theory

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Mean Force Kinetic Theory

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This talk will describe a recent approach to extend plasma kinetic theory into the strongly coupled regime [1]. The method is based on a new closure of the BBGKY hierarchy that expands about the deviations of correlations from their equilibrium values, rather than the strength of correlations. The model does not apply to arbitrary coupling strength because it still relies on the Markov approximation and a truncation of the hierarchy at second order in this expansion parameter. Nevertheless, it is found to extend the Boltzmann equation to orders of magnitude higher coupling strength. The result is a kinetic equation that is similar to the Boltzmann equation, but with three important distinctions: (1) The collision cross section is computed from particles interacting via the potential of mean force, rather than the bare Coulomb potential. This accounts for aspects of many-body physics in the interactions. (2) The spatial distribution of initial positions of interacting particles includes an excluded volume, similar to the Enskog theory for hard spheres, that is associated with short-range repulsion. (3) A term that is separate from the collision operator arises that is associated with capturing non-ideal equation of state properties consistent with classical statistical mechanics. The model has been tested by computing transport coefficients for hydrodynamic evolution of plasmas and comparing with molecular dynamics simulation and experimental results. Some of these comparisons will be reviewed. The general finding is that the approach extends plasma theory to Coulomb coupling parameters less than 10. The approach has also been applied to neutral fluids and has been shown to accurately extend the Boltzmann equation to the supercritical fluid regime for the Lennard-Jones fluid.

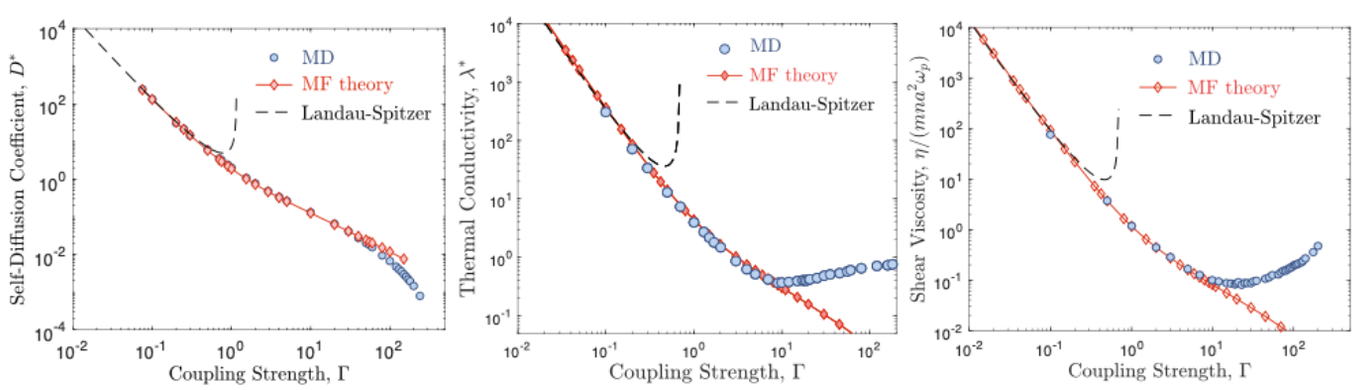

Figure 1: Comparison of molecular dynamics simulations, mean force kinetic theory, and traditional (Landau-Spiter) plasma theory for the self-diffusion (left), thermal conductivity (middle) and shear viscosity (right) of the one-component plasma. MD data from references [2-4].

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Waves in the medium and on the boundary of Quark-Gluon Plasma

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Quark-gluon plasma (QGP) is complex system of asymptotically freely moving particles of quarks and gluons in thermodynamic equilibrium [1]. The complexity of the many-body system demonstrates such collective properties that cannot be explained by the behaviour of single particles. For this reason, we study optical properties of the collective motion of partons, in particular, propagation of waves in the medium and on the boundary of QGP.

We plot dispersion relation to analyze oscillations in various phenomenological models. One of the model is collisional model that consider a system as weakly coupled plasma, which is described by kinetic equation with Bhatnagar–Gross–Krook (BGK) collision term [2]. However, recent RHIC results show that the matter in experiment is rather strongly coupled fluid. For that, we also consider viscous model that is derived from chromohydrodynamic equation with shear viscosity [3].

In order to study dispersion relation, we use dielectric functions of previously mentioned models. Investigation of waves in the medium requires solution of dispersion equation $\epsilon l(\omega,k) = 0$ for longitudinal modes. On the other hand, for waves on the boundary we have to solve [4]

$$\sqrt{\frac{k_z^2}{\omega^2} - 1} + \frac{2\omega}{\pi}\int_0^\infty \frac{dk_x}{k^2}\left(\frac{k_z^2}{\omega^2\epsilon_l} - \frac{k_x^2}{k^2 - \omega^2\epsilon_{tr}}\right) = 0$$

where, k2 = k2 + k2. To obtain this equation we consider a semi-infinite quark-gluon plasma which occupies half space region. So, we have a boundary at x-plane and and the plasma resides at the positive part of x-plane.

Finally, in this work we have compared dispersion relation for weakly coupled plasma and strongly coupled liquid regimes of QGP.

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Density Functional Theory calculations for high-temperature carbon plasmas

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Accurately modeling warm dense matter deep inside astrophysical objects is a great challenge. The associated thermodynamic states are characterized by solid-state densities, temperatures of thousands of Kelvin, and GPa pressures. The extreme of the conditions can vary gravely depending on the mass, radius, and composition of the studied object ranging from several GPa in planetary mantles to millions of GPa at the center of stellar interiors. A method that has proven highly successful in describing this peculiar state of matter is density functional theory molecular dynamics (DFT-MD). However, while the equations of states and transport properties for giant planets like Jupiter became increasingly accessible with DFT-MD simulations in the last two decades, extreme conditions as predicted for the interiors of low-mass stars seemed beyond reach.

In this talk, we discuss how DFT-MD calculations can be pushed to millions of Kelvin using carbon as an example. At very high densities, traditional DFT-MD codes based on plane- waves can be still used and we present a new ab initio approach to calculate the ionization degree based on the sum rule for the dynamic electrical conductivity [1]. At low densities and high temperatures, however, traditional plane-wave codes become intractable, because the number of partially occupied states increases significantly. This problem is addressed with the novel SQDFT code, which is a large-scale implementation of the Spectral Quadrature (SQ) method for O(N) Kohn-Sham DFT calculations [2,3]. The new capabilities of SQDFT are demonstrated for the Hugoniot curve for carbon up to 10 million Kelvin [4].

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The extended FPMD method for mid-Z materials

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The extended First-Principles Molecular Dynamics (ext. FPMD) method as implemented in the open source ABINIT code [1] is presented with a special emphasis on the calculation of the shift potential U0 that is at the heart of the process. The method is applied to materials of intermediate atomic number Z such as iron (Z=26) that suggests the use of different atomic datasets along an isochore, at contrast with low Z elements (hydrogen, boron, aluminum) where an all electrons pseudopotential can be used for the whole domain without any difficulty. We show how to account for the different atomic datasets and how to build an Hugoniot for iron up to Gigabar pressures that is compared with the previous calculations using QSCF code [2], Thomas-Fermi or SESAME #2140.

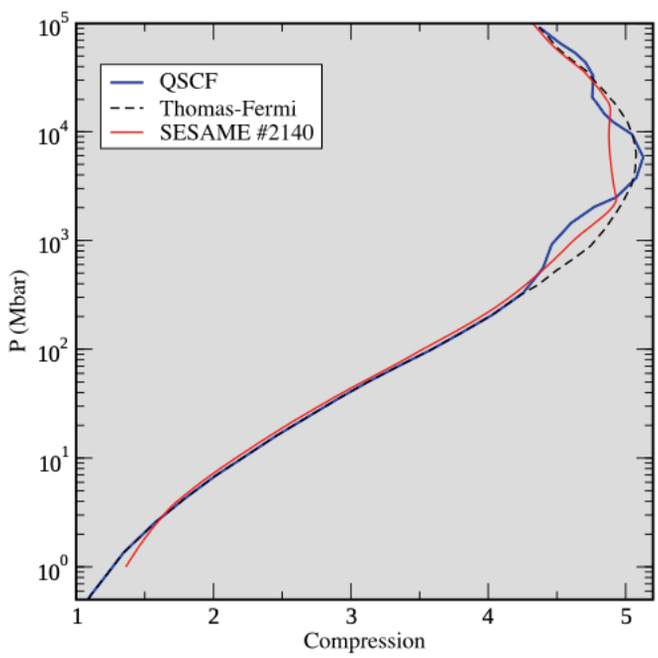

Figure 1: Hugoniot curve for Fe (p_0 = 7.85 g/cm3) obtained with QSCF model [2] (black solid line), SESAME #2140(red), and Thomas-Fermi (dashed line).

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Ab initio path integral Monte Carlo simulations of hydrogen snapshots at warm dense matter conditions

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We combine ab initio path integral Monte Carlo (PIMC) simulations with fixed ionic configurations, obtained by DFT-MD simulations, in order to solve the electronic problem for hydrogen under warm dense matter conditions. To solve the divergence problem in the Ewald-sum for attractive potentials we employ the pair-approximation. This approach is compared against the much simpler Kelbg pair-potential. We find very favorable convergence behavior towards the former. Since PIMC does not require any further assumptions regarding exchange and correlations of the many-body system, we then compare electronic densities obtained from our snapshot PIMC calculations with DFT calculations in the metallic regime. Furthermore, we investigate the manifestation of the resulting fermionic sign problem in our snapshot PIMC simulations. This gives us the unique capability to study the properties of warm dense hydrogen from ab initio simulations without any further assumptions, like the functional form of the exchange- correlation effects or fixed fermionic nodes. Thus, snapshot PIMC enables us to obtain the exact density response of warm dense hydrogen. This is extremely valuable to both experiments, like X-Ray Thomson scattering, as well as the development of new XC- functionals.

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Ultrafast dynamics of quantum many-body systems including dynamical screening and strong coupling

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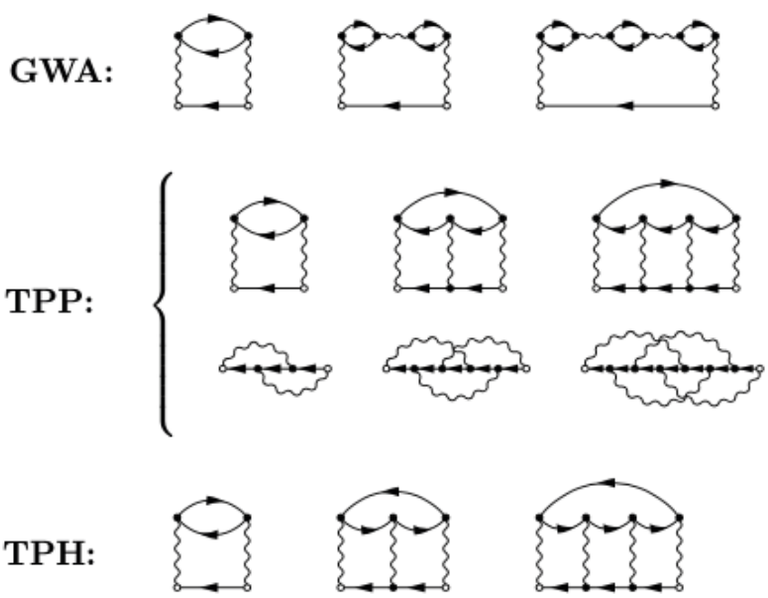
Dynamical screening is a key property of charged many-particle systems. Its theoretical description is based on the GW approximation (GWA) that is extensively applied for ground-state and equilibrium situations but also for systems driven out of equilibrium. The main limitation of the GW approximation is the neglect of strong electronic correlation effects that are important in many materials as well as in dense plasmas. Here we derive the dynamically screened ladder (DSL) approximation that selfconsistently includes, in addition to the GW diagrams, also particle–particle (TPP) and particle–hole T-matrix (TPH) diagrams, see figure. The derivation is based on reduced-density-operator theory [1] and the result is equivalent to the recently pre- sented G1–G2 scheme [2, 3] with three-particle correlations put equal to zero. We have performed extensive time-dependent DSL simulations for finite Hubbard clus- ters which confirm the excellent accuracy as well as total energy conservation of the approximation. At strong coupling and for long simulation durations, instabilities are observed. These problems are solved by enforcing contraction consistency and applying a purification approach [4].



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Thermalization of a beam of holes in a quasi-1D electron gas

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Quantum plasmas and electron-hole plasmas in nonequilibrium are successfully de- scribed using quantum kinetic theory and nonequilibrium Green functions (NEGF) [1]. Time-dependent expectation values of single-particle observables are accessi- ble via the one-particle NEGF. However, the propagation of the latter is computation- ally expensive, scaling with the number of time steps as Nt3. Recently, using the Gen- eralized Kadanoff-Baym Ansatz (GKBA) [2] with Hartree-Fock propagators this scal- ing could be drastically reduced to Nt3 → Nt1. The basis is the G1–G2 scheme [3,4] – an exact time-local reformulation of the GKBA. In this contribution we extend the G1–G2 scheme to a spatially uniform two-component system which we treat in mo- mentum representation. Due to the large dimension of the two-particle NEGF only a quasi-1D quantum wire geometry is feasible. To test the G1–G2 scheme we study the thermalization of a beam of positive charge carriers (holes, ions) injected into an electron gas along the wire axis. The equations are solved using second order Born selfenergies. Work on simulations using full nonequilibrium GW selfenergies is currently in progress.

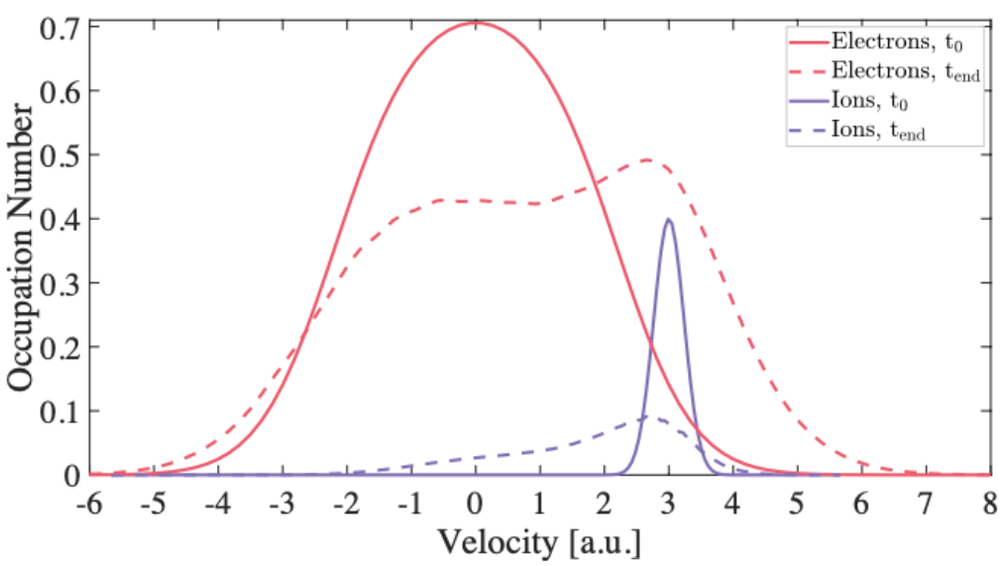

Figure 1: Time-resolved thermalization of an ion (hole) beam in a uniform quasi-1D electron gas.

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Ultradilute quantum liquid of dipolar atoms in a bilayer

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We show that ultradilute quantum liquids can be formed with ultracold bosonic dipolar atoms in a bilayer geometry. Contrary to previous realizations of ultradilute liquids, there is no need of stabilizing the system with an additional repulsive short-range potential. The advantage of the proposed system is that dipolar interactions on their own are sufficient for creation of a self-bound state and no additional short- range potential is needed for the stabilization. We perform quantum Monte Carlo simulations and find a rich ground state phase diagram that contains quantum phase transitions between liquid, solid, atomic gas, and molecular gas phases. The stabilization mechanism of the liquid phase is consistent with the microscopic scenario in which the effective dimer-dimer attraction is balanced by an effective three-dimer repulsion. The equilibrium density of the liquid, which is extremely small, can be controlled by the interlayer distance. From the equation of state, we extract the spinodal density, below which the homogeneous system breaks into droplets. Our results offer a new example of a two-dimensional interacting dipolar liquid in a clean and highly controllable setup [1].

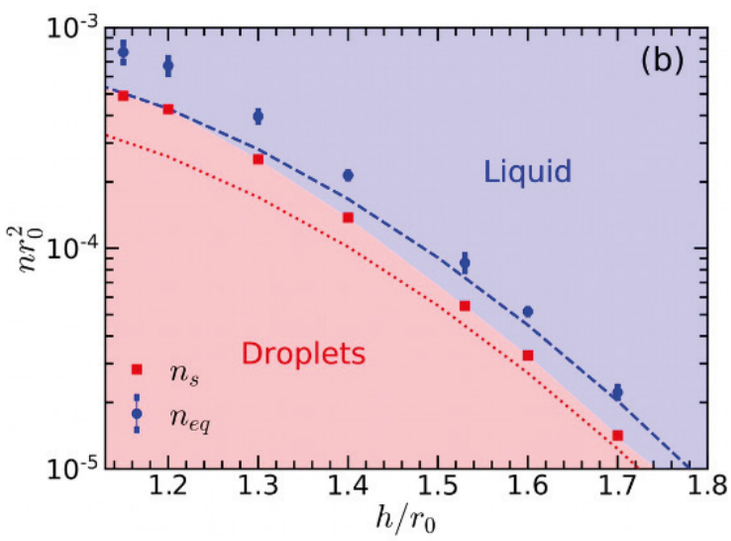

Figure 1: Phase diagram of the dipolar liquid phase

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Accurate and efficient calculations of mean ionization states with an average-atom model

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The mean ionization state (MIS) is a critical property in dense plasma and warm dense matter research. It is used (for example) as an input parameter in various models, including for example the calculation of adiabats in inertial confinement fusion; it is also used to help interpret and fit experimental results. Unfortunately however, theoretical predictions of the MIS are often inconsistent with each other and experimental data. In this presentation, I will compute the MIS using a variety of approaches in an average-atom model and compare results with higher-fidelity simulations and experimental benchmarks [1]. I will show that the canonical approach for computing the MIS is usually insufficient; I will also discuss a novel approach based on the electron localization function, which yields improved results but tends to systematically under-estimate the MIS. Finally, I will adapt a recently-proposed Kubo–Greenwood method [2] to our computationally efficient average-atom model, which shows very promising agreement with all the benchmarks considered, with one example shown in Fig. 1 below.

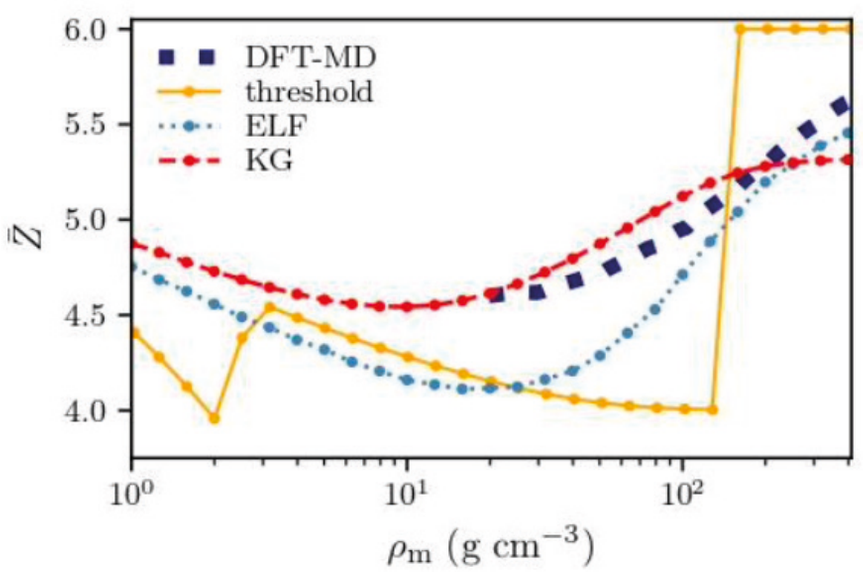

Figure 1: Mean ionization state comparisons for Carbon as a function of density, for fixed temperature T=100 eV. The Kubo–Greenwood (KG) method applied to our average-atom model yields excellent agreement with the DFT-MD benchmark.

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Data-Driven and Physics-Informed Modeling of Matter under Extreme Conditions

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The successful characterization of high energy density (HED) phenomena in laboratories using pulsed power facilities and coherent light sources is possible only with numerical modeling for design, diagnostic development, and data interpretation. The persistence of electron correlation in HED matter is one of the greatest challenges for accurate numerical modeling and has hitherto impeded our ability to model HED phenomena across multiple length and time scales at sufficient accuracy. Standard methods from electronic structure theory capture electron correlation at high accuracy, but are limited to small scales due to their high computational cost.

The use of machine-learning techniques, and in particular, deep neural networks, has become the standard in many research areas, but their full potential remains yet to be exploited in materials science. Their potential to reduce computational cost and provide novel physical insights is becoming increasingly relevant in current scientific practice [1].

In this talk, I will summarize our recent efforts on devising a data-driven and physics- informed workflow to tackle this challenge. Based on first-principles data we generate machine-learning surrogate models that replace traditional density functional theory calculations [2]. Our surrogates predict the electronic structure and related properties of matter under extreme conditions highly efficiently while maintaining the accuracy of traditional methods [3].

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Sensitivity of uniaxially driven ICF target performance to interfacial conduction in the high-energy-density regime

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First Light Fusion (FLF) is a private UK company investigating a novel approach to inertial fusion energy (IFE), through means of hyper-velocity projectile-driven impact. Some of the most useful insights into the necessary physics in a configuration of direct relevance to FLF's recent research are due to the experiments of Derentowicz et al. [1], which used shaped charges to produce TPa-pressure Mach waves for collapsing D2-filled conical cavities in an Au anvil. Initial modelling of this system has shown it to be a physics-rich system, with an unexpected degree of sensitivity to the modelling of thermal conduction, especially at the fuel-anvil interface, and the associated plasma microphysics [2].

Unlike laser-plasma systems, the transient shock-driven temperature separation created in such targets leads to a situation in which both electronic and ionic thermal conduction contribute strongly to the energy loss from the thermonuclear fuel. Of particular importance is the way heat is transported through the interface between the fuel and the anvil. Furthermore, our work has suggested that non-local ionic conduction may also become important. Uncertainties in the modelling of these quantities therefore has a substantial impact on predicted target performance.

In this submission, we will present our most recent results from detailed multivariate sensitivity studies of the Derandomize-type target using Hytrac; one of FLF's in-house radiation-hydrodynamic IFE design codes. The results support our earlier conclusions [2]: specifically, the averaging method used to approximate flux-limited thermal conduction at the fuel-anvil interface, which occurs between a classical high-temperature deuterium plasma and gold at near-solid density and a few eV. To focus on the relevant physics in a similar geometry, but without the uncertainty associated with non-local effects, we have performed a similar study based on the conically convergent shock tube experiments of Setchell et al. [3]. These results further strengthen the importance of interfacial conduction modelling. Finally, we show the first results from an ongoing collaboration in which reduced kinetic modelling enables more accurate representation of the ionic heat flux in the non-local regime.

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Dynamical formation of the Diamond rain in icy giant planets by C-H immiscibility

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The accumulation and circulation of carbon and hydrogen dictate the chemical evolution of ice giant planets [1-2]. Species separation and diamond precipitation have been reported in carbon–hydrogen systems, as verified by static and shock compression experiments [3-4]. Nevertheless, the dynamic formation processes for the above-mentioned phenomena are still insufficient and poorly understood. Here, we demonstrate that diamonds form through a three-step process involving decomposition, species separation and nucleation procedures. Under shock condition of 125 GPa and 4590 K, hydrocarbons are decomposed to give hydrogen and low- molecular-weight alkanes (CH4 and C2H6), which escape from the carbon chains resulting in C/H species separation. The remaining carbon atoms without C–H bonds accumulate and nucleate to form diamond crystals. The process of diamond growth is found to associated with a critical nucleus size where dynamic energy barrier plays a key role. These dynamic processes for diamonds formation are insightful in establishing the model for ice giant planet evolution.

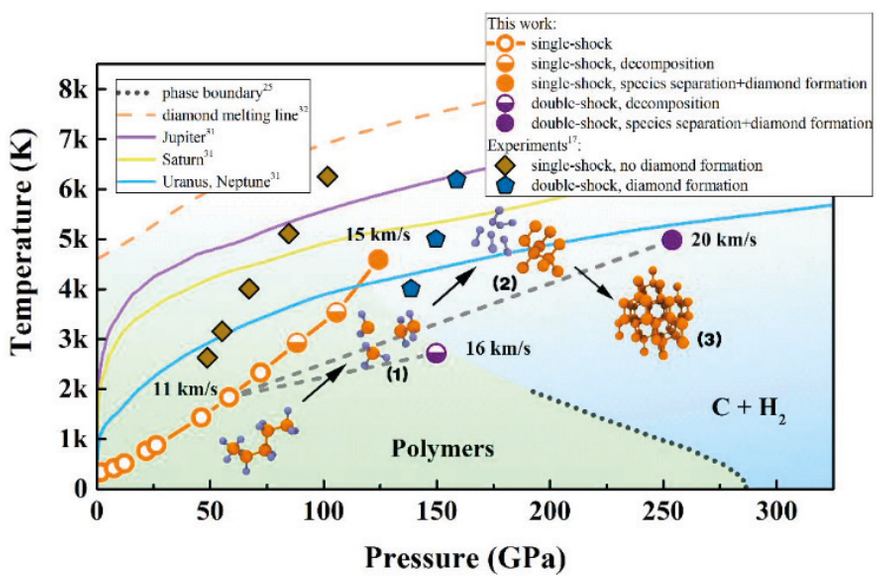

Figure 1: Summary of thermodynamic conditions and formation processes of diamonds in Shock-compressed Hydrocarbons.

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How 2D solid loses its structural order in the KTHNY melting transition through defect excitation

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It is widely accepted that the melting transition governed by the Kosterlitz-Thouless- Halperin-Nelson-Young theory [1,2,3] is a two-stage transition through the intermediate hexatic phase. The pair generation and separation of dislocation defects have been demonstrated as the causes for the loss of translational order by various numerical simulations [4]. However, the spatiotemporal behaviors of topological defects in the solid close to the hexatic phase still remain elusive. Here, this issue is numerically addressed by using a 2D Yukawa system heated to nearby the hexatic point. It is found that the thermally excited collective particle motions cause lattice wiggling and distortion, which in turn generate dislocation defects through bond breaking/reconnection. The successive generation, traveling, interaction, annihilation of dislocation defects under the conservation of Burgers vector, can lead to the intermittent emerging of local crystalline ordered domains with different lattice orientations, surrounded by dislocation defect strings.

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Monte Carlo results for quantum Hall liquid crystalline phases of electrons

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Strongly correlated two-dimensional Coulomb systems especially those subject to a strong perpendicular magnetic field exhibit some of the most intriguing phenomena in condensed matter physics. The interplay between magnetic field and strong Coulomb interactions can drive such systems into novel quantum phases that cannot be described by standard paradigms. Notable examples are the integer and fractional quantum Hall phases that stabilize under specific conditions. In this work, we investigate possible liquid crystalline phases of electrons that may be observed at certain even-denominator filling factors of a quantum Hall system. These phases are described by a broken rotational symmetry wave function with inherent anisotropy. Results obtained from Monte Carlo simulations of finite systems of electrons in disk geometry are presented.

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Carbon ionization in the hot dense regime

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The determination of the ionization of a system in a hot dense regime is an old question which has been revived by recent results. We propose here an evaluation of the ionization based on the structure of the plasma, valid for temperatures above 50 eV. Using the extended method [1], we performed simulations along the 100 eV carbon isotherm (Fig. 1) with a sufficient number of particles (32 to 64) to obtain well- converged pair distribution functions (PDF). By matching the PDF with the one of a one-componentplasma(OCP),onecandefineanionizationQS bythestructurewhich turns out to be in good agreement with a definition QP by the pressure. These values are compared to the results from two quantum average-atom codes. The first one (SCAALP_OCP [2]) takes into account for a ionic structure using the OCP reference system, while the second one (QAAM [3]) is based on the muffin-tin approximation. We also extracted the ionization from SQDFT [4] simulations along the 10 g/cm3 carbon isochor between 8.6 and 860 eV (Fig. 2). The two estimates QS and QP are in very good agreement with each other in both cases (isothermal and isochoric). At low temperature Qs and Qp are lower than the average-atom calculations. We suspect that these differences correspond to the appearance of atomic bonds in the system.

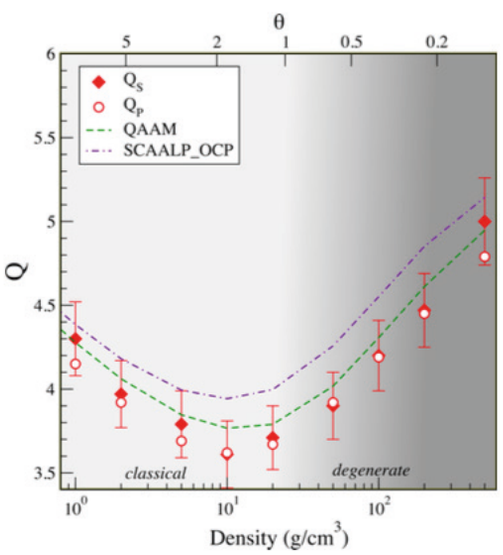

Figure 1: Ionization of carbon along the 100 eV isotherm. Symbols are extended FPMD simulations and dashed lines are average-atom calculations.

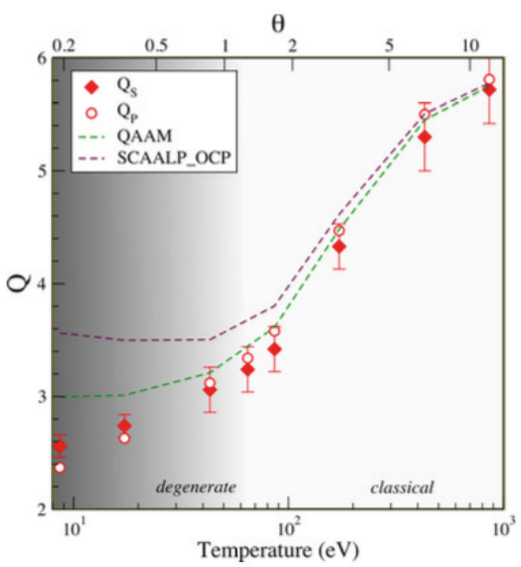

Figure 2: Ionization of carbon along the 10 g/cm3 isochor. Symbols are SQDFT simulations and dashed lines average-atom calculations.

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Stochastic Representation of Many-Body Quantum States

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The quantum many-body problem is ultimately a curse of dimensionality: the state of a system with many particles is determined by a function with many dimensions, which rapidly becomes difficult to efficiently store, evaluate and manipulate numerically. On the other hand, modern machine learning models like deep neural networks can express highly correlated functions in extremely large-dimensional spaces, including those describing quantum mechanical problems. We show that if one represents wavefunctions as a stochastically generated set of sample points, the problem of finding ground states can be reduced to one where the most technically challenging step is that of performing regression—a standard supervised learning task. Remarkably, in the stochastic representation the (anti)symmetric property of fermionic/bosonic wavefunction can be used for data augmentation and learned rather than explicitly enforced. We further demonstrate that propagation of an ansatz towards the ground state can then be performed in a more robust and computationally scalable fashion than traditional variational approaches allow.

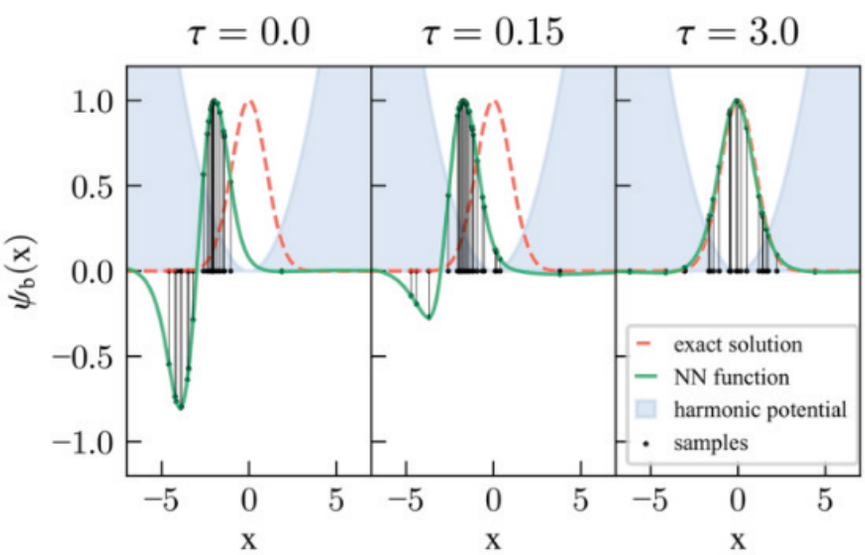

Figure 1: Different steps in the propagation towards the ground state of a particle of mass m=1 in a 1D harmonic oscillator with frequency =1, with ħ=1. The green line is the function fitted by the NN to a finite set of samples (black dots on the x-axis) and their corresponding values (connected by a black line). Starting with an assymetric guess (τ=0), the function converges towards the correct solution (dotted orange line) at the center of the trap and acquires the right symmetry (τ=3).

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Exciton supersolid phase transition in bilayer semiconductors

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We predict a stable supersolid ground state of spatially indirect excitons. In this supersolid phase, with exactly one exciton per lattice site, there is translational symmetry of the exciton crystal and, simultaneously, phase coherence of the exciton condensate [1].

The electrons and holes of the excitons are confined in spatially separated layers of a semiconductor heterostructure. For small layer separations, superfluid condensation of excitons has already been demonstrated in bilayer semiconductors [2-5].

We use a variational approach to establish the ground state phase diagram, with layer separation (d) and exciton density (n) as parameters. Ref. [6] had predicted with dipolar interactions, that at large layer separations there is a phase transition from exciton liquid to exciton normal solid (EL-ENS). However, we find a superfluid to supersolid phase transition at much lower d, and that the supersolid persists up to d larger than the predicted EL-ENS transition, before a second phase transition from supersolid to ENS.

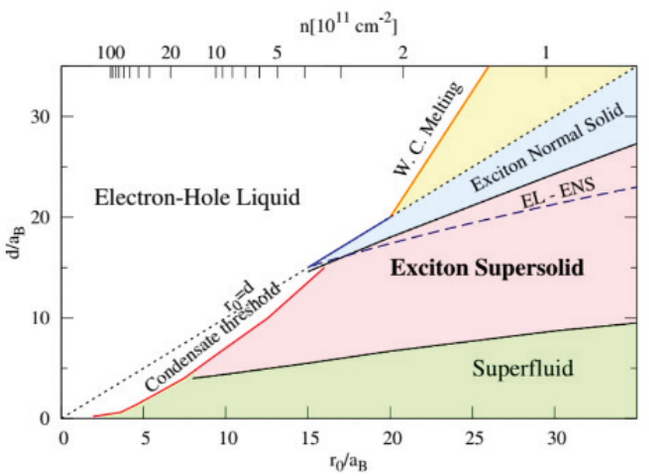

Figure 1: Phase diagram(T=0). d: layer separation; r0 characterizes the density n.

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Generalized chemical model for ionization and dissociation in warm dense hydrogen

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To evaluate the thermodynamic and transport properties of warm dense matter [1], computer simulation methods are widely used, including the method of molecular dynamics with semiclassical interaction potentials, quantum versions of the Monte Carlo method and of molecular dynamics, as well as various approximations of the wave packet molecular dynamics. In addition, the density functional theory is extensively applied in order to simultaneously take into account both the plasma component and the presence of strongly coupled ions. It should be noted that all the mentioned simulation techniques provide a very high degree of accuracy but at the same time require a substantial computational time [2-4].

In this poster, to comprehensively study warm dense hydrogen, containing electrons, ions, neutral atoms and molecules, a generalized chemical model [5] is consistently utilized, which makes it possible to calculate both the lowering of the ionization potential of atoms due to the interparticle interactions in the medium and the corresponding change in the dissociation energy of molecules. At the same time, since the effective macroscopic potential is central to the entire consideration, this provides an unprecedented opportunity to simultaneously determine the thermodynamic and transport properties of warm dense hydrogen, which cannot be achieved within the framework of other existing approaches.

The behavior of the ionization degree of atoms and the dissociation degree of hydrogen molecules are both determined in a very broad range of plasma parameters and a thorough comparison is made with the available data of both computer simulations and real experiments.

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Excitonic condensation, pairing gap and quadri-excitons in an electron-hole bilayer with twofold valley degeneracy

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We study a model of symmetric electron-hole bilayer, encoding the key features, valley degeneracy and many-body correlations, of coupled graphene bilayers separated by a thin insulating material. Using Quantum Monte Carlo simulations we map the phase diagram of our model in the plane carrier density/ bilayer separation.
We found an excitonic phase (bound pairs of opposite charges) sandwiched between a plasma phase and a quadriexcitonic phase (characterised by complexes of eight-particles) [1]. We calculate the condensate fraction, pair correlation functions and the pairing gap to characterise the phases of the model.
Only the intermediate excitonic phase undergoes Bose-Einstein condensation, possibly explaining why anomalous tunnelling conductivity, interpreted as signature of condensation, is observed only between two finite values of carrier density in graphene bilayers [2].

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The physics of liquid carbon, and evidence for possible superionic C, H mixtures in the low-temperature warm-dense-fluid regime

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Carbon, the third most-abundant element in the universe forms a metallic fluid with transient-covalent bonds (TCBs). Its liquid-liquid phase transitions (LPTs), extensively sought using the TCB paradigm had remained elusive. We have shown [1], using two independent DFT methods that liquid carbon displays multiple LPTs in the density (ρ) range 2.9 g/cm3 to 6.0 g/cm3 when a coordination number of 12 is reached. This property holds for temperatures T < 4 eV for this density range where the Fermi energy EF is very high (> 25eV). The structure factor splits to create a subpeak tied to twice the Fermi wavevector (kF), constraining the fluid structure in momentum space as in a charge-density wave, to take energetic advantage of the strong scattering of electons by ions from one edge of the Fermi surface to its opposite edge valid at low T/EF. The resulting dominent Friedel oscillations of the C-C interaction obtained within a metallic-liquid paradigm favour liquid-liquid transitons on change of the coordination number, a property possibly shared by other similar metallic `tetrahedral' fluids like Si and Ge [2,3]. The hold on the ionic structure by the $2k_F$ scattering is so strong that on addition of hydrogen to the system in this regime of ρ and T, the fluid structure remains largely unchanged, and the protons form a nearly independent subsystem showing superionic behaviour. At sufficiently high temperatures the Friedel control of the ionic structure is lost and the system reverts to a standard mixture of interacting ions and electrons. These results are critical to terrestrial and astrophysical studies where C, H systems are ubiquitious, and to the search for emerging new carbon materials .

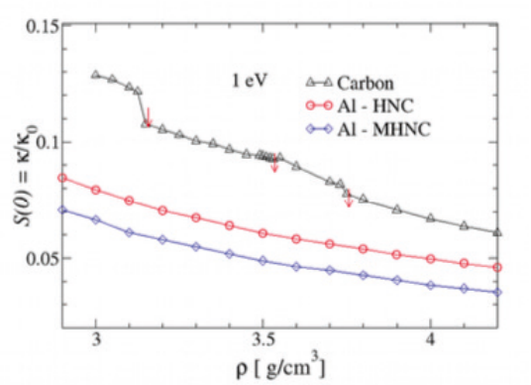

Figure 1: Discontinuities in the compressibility of liquid carbon contrasted with that of lqd. Al. See Ref. [1] for details.

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Soliton propagation and trapping in a 2D dusty plasma layer

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The propagation of solitons is investigated in a 2D dusty plasma layer (modelled as a Yukawa liquid), via molecular dynamics simulations comprising 4x106 particles. Density perturbations are created in an equilibrated system by an electric field pulse having a Gaussian shape in space and a short duration (less than a plasma oscillation period) in time [1]. Such pulses generate pairs of solitons, which are characterized by a positive and a negative density peak, which propagate into opposite directions. At small amplitudes of the perturbation, these features propagate with the longitudinal sound speed, from which an increasing deviation is found at higher perturbations. An external static magnetic field, oriented perpendicular to the layer of the system blocks the propagation of the solitons, which can, however, be released upon the termination of the magnetic field and can propagate further into directions that depend on the time of trapping and the magnetic field strength [1]. Figure 1 illustrates the propagation of solitons for the coupling and screening parameters Γ= 100 and κ = 1, in the unmagnetized case (left panel) and in a case where the magnetic field is turned on during the simulation (right panel).

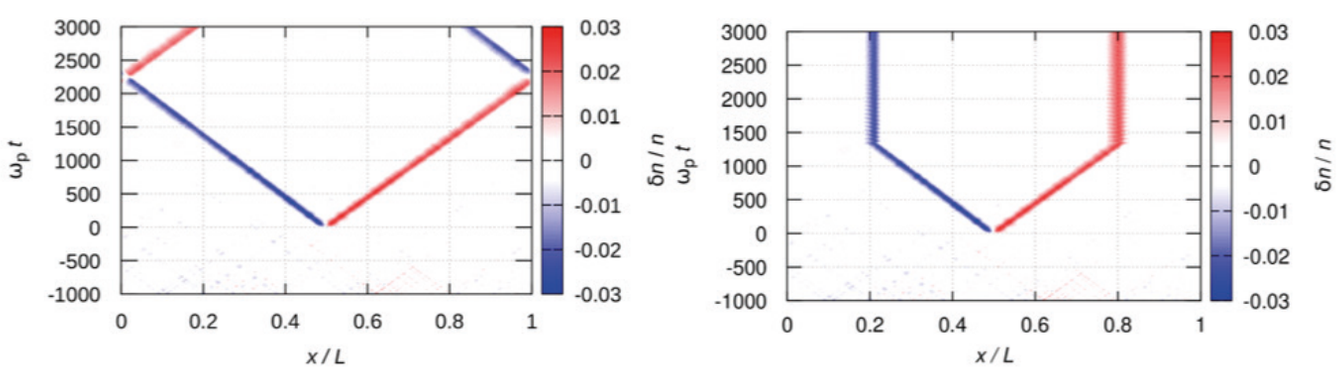

Figure 1: Density perturbation in the system as compared to homogeneous density as a function of space and time (position is normalized with the size of the computational domain; time is normalized by the inverse plasma frequency). The perturbing electric field is applied at t = 0, at the centre of the domain. Solitons that leave the simulation box at either side, re-enter the box at the opposite side, according to the periodic boundary conditions. Left panel: unmagnetized system, right panel: a perpendicular magnetic field is turned on at time wp t = 1333.3. Negative values of time correspond to the equilibration phase of the simulation.

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Electronic pair alignment and roton feature in the warm dense electron gas

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The study of matter under extreme densities and temperatures as they occur e.g. in astrophysical objects and nuclear fusion applications has emerged as one of the most active frontiers in physics, material science, and related disciplines. In this context, a key quantity is given by the dynamic structure factor S(q,ω), which is probed in scattering experiments -- the most widely used method of diagnostics at these extreme conditions. In addition to its crucial importance for the study of warm dense matter, the modeling of such dynamic properties of correlated quantum many- body systems constitutes one of the most fundamental theoretical challenges of our time. Here we report a hitherto unexplained roton feature in S(q,ω) of the warm dense electron gas [1], and introduce a microscopic explanation in terms of a new electronic pair alignment model [2]. This new paradigm will be highly important for the understanding of warm dense matter, and has a direct impact on the interpretation of scattering experiments. Moreover, we expect our results to give unprecedented insights into the dynamics of a number of correlated quantum many- body systems such as ultracold helium, dipolar supersolids, and bilayer heterostructures.

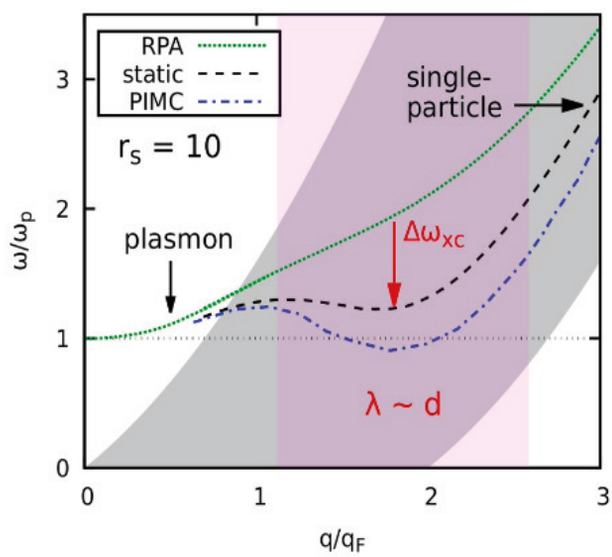

Figure 1: Spectrum of density fluctuations [maximum in the dynamic structure factor S(q,ω)] of the UEG at the electronic Fermi temperature. Green: random phase approximation; black: static approximation [1]; blue: exact PIMC results [1]. The roton minimum at λ ~ d is a consequence of the down-shift Δωxc compared to RPA due to the alignment of electron pairs [2].

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Electron–atom interaction in dense plasma of noble gases

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Collisional processes determine practically all the properties of the plasma, its composition, thermodynamics, transport characteristics, electrodynamic properties, etc. Therefore, it is important to carry out studies correctly and reliably at the level of elementary processes. The study of interaction potentials of particles and their collisional properties is one of the most important areas of plasma physics. At present, due to the important role of transport processes both in the plasma of technical devices (thermonuclear fusion, medicine, etc.) and in natural systems (astrophysics, etc.), this branch of plasma physics continues to develop.

In this paper, we considered the collision of electrons with atoms of noble gases. The effective potential of the optical interaction was used to describe the pairwise interaction of an electron with an atom. This optical potential takes into account the effect of diffraction at short distances and the effect of screening at large distances [1-3].

The authors are grateful to the Science Committee of the Ministry of Education and Science of the Republic of Kazakhstan for their support under grant No. AP08855972.

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Investigation of the fluctuation-theorem convergence in a dusty plasma experiment

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In this talk, I will present our recent discovery in non-equilibrium statistical mechanics using a dusty plasma experiment.
In the laboratory conditions, micron-sized dust particles are negatively charged to thousands to tens of thousands elementary charges. As a result, these dust particles are strongly coupled, arranging themselves like atoms/molecules in liquids or solids. During experiments, these dust particles can directly recorded using video imaging, and then their motion can be tracked individually in the data analysis. Thus, from experiments one may directly obtain positions and velocities of dust particles, which can be used to test theories of statistical physics. Here, we report a shear-induced melting dusty plasma experiment [1, 2], where two counter propagating flows are generated by two oppositely directed laser beams. Between these two flows, we choose different subsystems with various sizes, containing from 6 to 62 particles in average. Using the observed particle positions and velocities in our experiment, we calculate the time series of the entropy production rate for various subsystems. For various subsystems, it is found that the distribution of the averaged entropy production rate can be fit to the Gaussian function quite well [2]. Using the Gaussian distribution entropy production rate, we derive the analytical expression of the asymptotic trend of our experimental data to the SSFT. Based on these obtained data, we find that, as the subsystem size increases gradually, the SSFT convergence times diminishes gradually until reaching its minimum, which is just the Maxwell relaxation time. Using our Langevin simulations, these findings are further verified by a wider range of the subsystem size. We interpret the observed minimum convergence time as a consequence of the elastic properties in the viscoelasticity of the studied dusty plasma system.

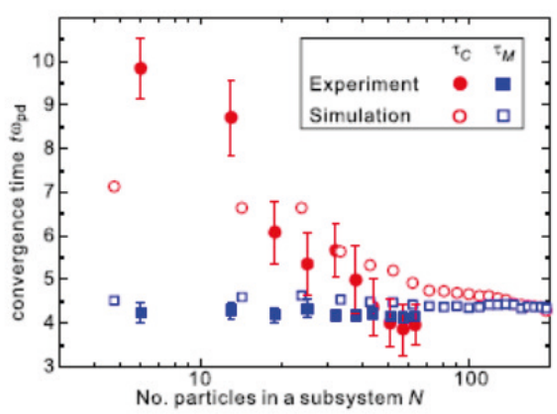

Figure 1: Obtained convergence time while varying the analyzed subsystem size.

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Transferability of DFT surrogate models: Temperature and system size

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While Density Functional Theory (DFT) is the most common tool for the investigation of materials under extreme conditions, its scaling behavior with respect to both system size and temperature makes large scale simulations challenging. Yet, progress in this regard would enable accurate modeling of planetary interiors or radiation damage in fusion reactor walls.
One possible route to alleviate these scaling problems is through the use of surrogate models, i.e., machine-learning models. These are trained on DFT data and are able to reproduce DFT observables at comparable accuracy, but negligible computational cost.
In order to actually be useful for such investigations, existing models need to be able to work across length scales and be transferable within desired temperature ranges. Here we show how models based on local mappings of electronic structure information [1], implemented in the Materials Learning Algorithms (MALA) package [2] can be trained on small number of atoms and select temperatures, yet perform accurately when used to make predictions for extended systems within a range of temperatures.

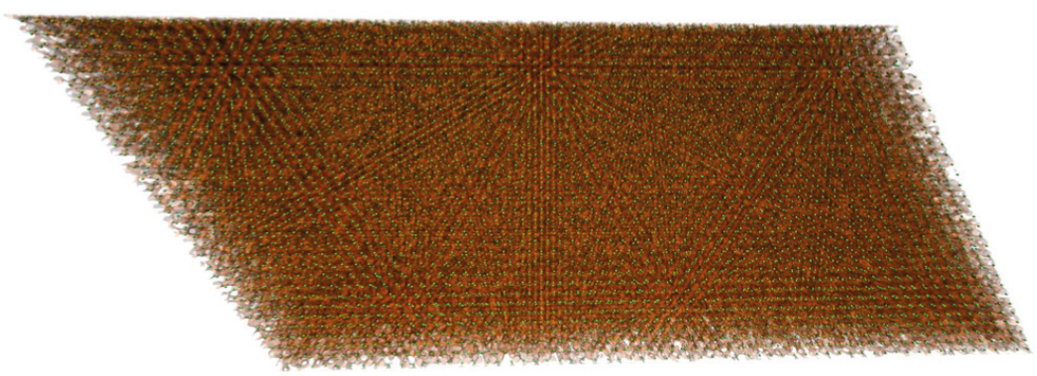

Figure 1: Electronic density of 131072 beryllium atoms, predicted with MALA [2].

[1]: J. A. Ellis et al., Phys. Rev. B 104, 035120, 2021
[2]: https://github.com/mala-project

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Supersolid state of a dilute exciton gas in electron-hole bilayers

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Using the coherent-state wave function formalism (the Keldysh formalism), developed with reference to a bilayer electron-hole system [1] (see also [2] for a review), we describe the transition to the supersolid state in a two-dimensional dilute condensate of electron-hole pairs with spatially separated components. The appearance of a roton-type minimum in the collective excitation spectrum signals the instability of the system with respect to the thansition to the state with spatial modulation of the condensate. It is found that it is the first-order transition to a hexagonal supersolid phase [3] (Fig.1). It has been shown that there is a jump in the average density of the condensate during the phase transition. It is also shown that the formation of a complicate "ship" wave pattern under the
flow of the uniform condensate of electron-hole pairs past a point obstacle can be considered as a precursor of the transition to the supersolid state [4] (Fig. 2).

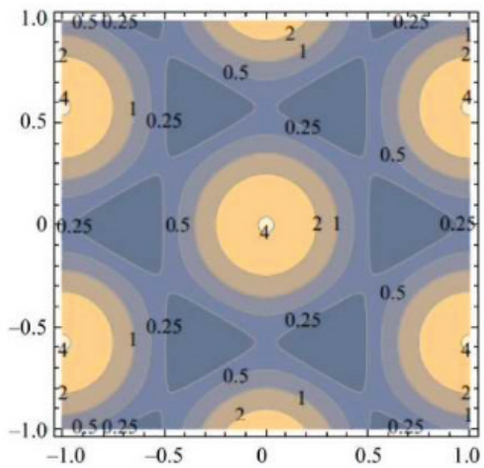

Figure 1: Distribution of the condensate density in the supersolid state near the transition line.

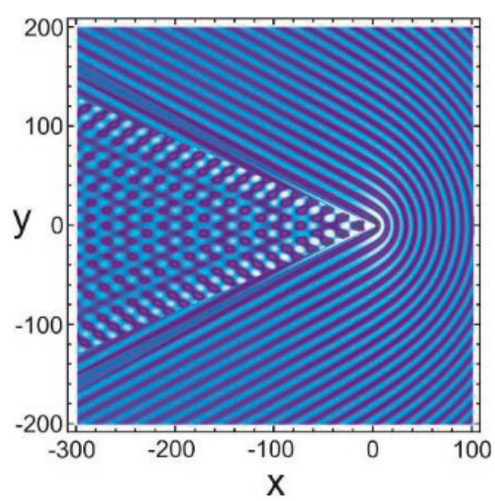

Figure 2: An example of the "ship" wave pattern in the uniform state near the transition line. The unit of length is the effective Bohr radius.

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Electronic transport coefficients of hydrogen from density functional theory across the plasma plane

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Density functional theory (DFT) is a widely used method to efficiently describe strongly coupled Coulomb systems on a quantum-mechanical basis. While formally designed to reproduce energy and other equilibrium properties of the Coulomb system, it can also be employed to calculate transport coefficients like the electrical and thermal conductivity. This is possible via the Kubo-Greenwood formalism [1], which has been successfully applied to several liquid and solid metals and other elements in the plasma state.

An open question that has, so far, been discussed controversially is whether or not the mean-field description of electrons in DFT can accurately account for electron- electron scattering process [2]. This question can be answered by calculating electronic transport coefficients in the weakly coupled and weakly degenerate region, where limiting values have been established by kinetic theory. However, such conditions are highly challenging from the computational point of view because a large number of particles and bands need to be calculated in the DFT.

Here we present results from DFT calculations for hydrogen plasmas that span a wide range of states across the plasma plane. By comparing thermopower and Lorenz number with their respective limiting values provided by the Spitzer theory [3], we show that electron-electron scattering processes are not accounted for in the usual combination of DFT with the Kubo-Greenwood formalism [4]. This necessitates further improvement of the theoretical description, probably to an explicit two-particle level.

Our findings are of substantial importance for future methodical developments to calculate transport properties of Coulomb systems and, especially, for correctly assessing the results obtained via the Kubo-Greenwood formalism in relation to experiments and other theoretical approaches.
This work was supported by the Deutsche Forschungsgemeinschaft (DFG) within the FOR 2440. The DFT calculations were performed at the North-German Super- computing Alliance (HLRN) facilities.

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[4] M. French, G. Röpke, M. Schörner, M. Bethkenhagen, M. P. Desjarlais, and R. Redmer, submitted (2022).

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Ab initio plasmon dispersion of the warm electron gas

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The plasmon dispersion ω(q) and damping γ(q) contain important information on the state of warm dense matter. On the other hand, x-ray Thomson scattering (XRTS) experiments provide accurate data for the dynamic structure factor S(q,ω) that is directly linked to the plasmon spectrum [1]. However, details of this link depend on the quality of the theoretical model for the dielectric function. Here we present the first ab initio data for the dielectric function that is obtained by quantum Monte Carlo simulations [2]. This allows us to obtain high quality results for ω(q) and γ(q) of the electron component at warm dense matter conditions. Second, we critically analyze the commonly used weak damping approximation for the dispersion and improve it by performing the analytic continuation of the dielectric function. This yields results that apply at strong damping and large wave numbers as well, which is the basis for a more accurate comparison with XRTS experiments [4].

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Microfluidic flow in single-layer dusty plasmas

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Experiments on strongly coupled dusty plasmas provide unique access to the microscopic details of macroscopic processes in condensed matter. Since the early years of this field, the application to hydro- dynamic processes was one of the main motivations. In most cases, however, the complexities of the experiments prevented the drawing of universal conclusions. At the same time, single layer dusty plasma crystals produced in plane-parallel RF discharges became the main subject of most laboratory dusty plasma experiments, because this configuration provides best control of plasma parameters and reproducibility of the results.

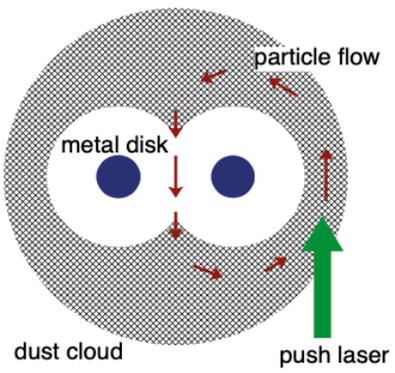

Figure 1: Sketch of the top view.

We investigate hydrodynamic flows in a complex plasma by utilizing the control provided by the plane-parallel RF discharge configuration. Two metallic disks are placed on the powered electrode of the new, large area (16" diameter) dusty plasma experiment at the CASPER Lab, forming an electrostatic potential channel. Dust particle flow through the channel is induced by indirect laser manipulation as shown in figure 1. By adjusting the argon gas pressure and RF power, the channel could be tuned to allow the formation of single or multiple lanes of transiting dust particles. We use this system to address fundamental details of hydrodynamic flows like the acceleration and stopping of particles, lane formation and ordering in the channel as visualized in figure 2.

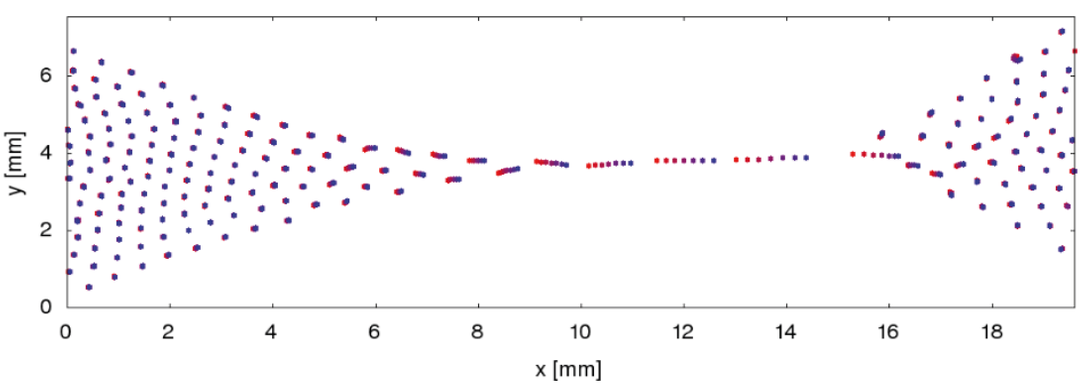

Figure 2: Top view. Color coded time-evolution of a single-lane particle flow with 60 fps resolution.

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Emergent Coulomb Fluids in Spin Ice

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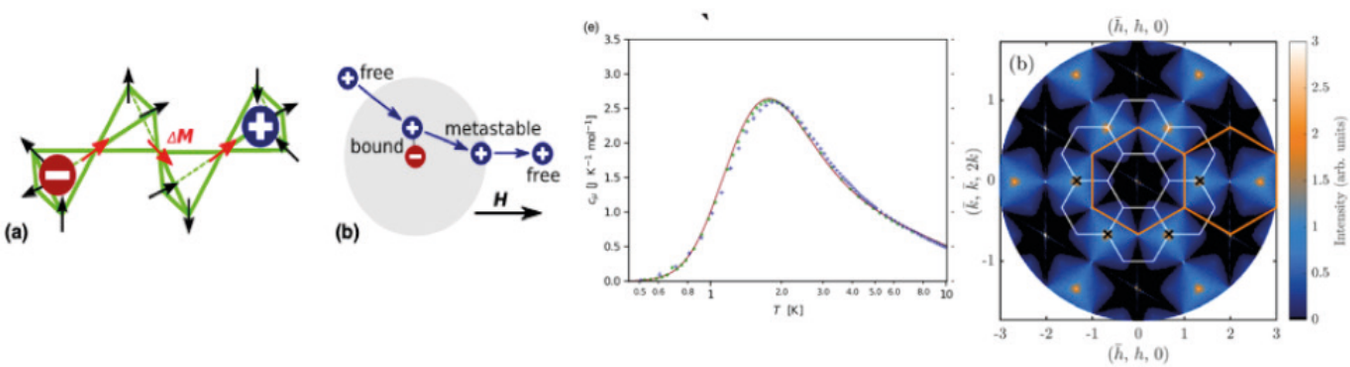
The quasi particle excitations of the frustrated magnets known as spin ice are topological defects carrying magnetic charge – magnetic monopoles [1,2]. As a consequence, spin ice can be treated, to an excellent approximation as a magnetic Coulomb fluid in the grand canonical ensemble. In this emergent description the magnetic moments play the role of elements of a lattice field describing the emergent magnetostatics. This duel description - a particle, or field theoretic point of view - gives access to thermodynamic [3] and dynamic [4] properties as well as to magnetic correlations [5].
In this seminar I will review the Coulomb fluid physics of spin ice including specific heat via Debye-Hückel-Bjerrum theory, monopole crystallization, Onsager's Wein effect and Coulomb phase pinch point scattering patterns.



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Fast Simulations of Complex Charged Systems for Soft Matter Applications

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In this talk I will present various algorithms to treat Coulomb interactions for soft matter systems and discuss some exemplary applications. I start with presenting an investigation of various Coulomb solvers implemented in ScaFaCoS [1], a parallel scalable library for Coulomb interactions in particle systems, and compare them with respect to complexity, scalability, performance, and accuracy. To ensure comparable conditions for all methods and to cover typical applications, we tested all methods on the same set of computers using identical benchmark systems. For soft matter systems it turned out that Fast Multipole methods and FFT-based mesh Ewald methods were the most efficient ones in performance and stability. Since models for soft matter systems mostly use the implicit solvent approximation, solvents are characterized by their relative dielectric constant. This, in turn, can introduce dielectric discontinuities at boundaries to solid materials [2,3], or even locally varying dielectric responses [4,5] can occur in electrolytes of varying salt density. In the following I will discuss various ways of handling those more complicated boundary conditions for fast Coulomb solvers, and present some physical implications of such complications. At last, I will discuss implications of constant potential boundary conditions, as they are important for supercapacitor applications and electrochemical batterie applications [6], and talk shortly about our open-source molecular dynamics package ESPResSo [7] that contains all of the presented algorithms.

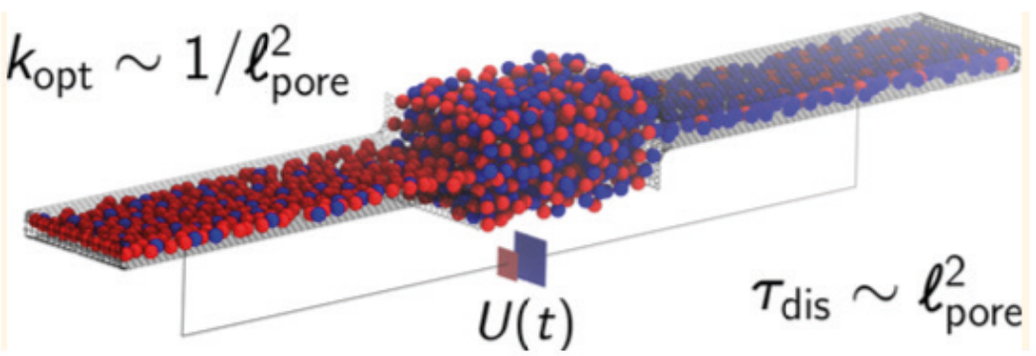

Figure 1: Snapshot of a slite pore under constant potencial conditions containing a model electrolyte [6].

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Enhancement of electron-impact ionization induced by warm dense environments

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With the development of laser technology, the electron-impact ionization process in warm dense matter could be studied by using ultra-intense lasers in the laboratory, which is crucial for both fundamental science and practical applications in modeling of concepts in astrophysics and laboratory plasmas. However, the measurement of Berg et al. [1], which studied how charge states generated using electron-impact ionization process via resonance pumping of the 1s-2p transition significantly differs from theoretical calculations on the electron-impact ionization cross section in warm dense matter. The experimental result is larger than the predicted values from the standard atomic collision theory, which provides some new insights into ionization in warm dense matter.

For the theoretical results are based on structures of the isolated atoms of ions, without considering the influence of hot dense plasmas, we present a model to consider the effects of the ion and free electrons in the self-consistently calculations of ionic structures, and free electrons decoherence in the electron-impact ionization. The correlation effects due to the interactions between ions and surrounding free electrons, are included by the correlation functions, which are calculated by hyper-netted chain (HNC) approximation. And the effect yields an additional Hermitian potential to the atomic central potential, and will significantly change the atomic structure compared with that of the isolated ion. Due to the partial decoherence caused by random collision with free electrons and ions, we use damped plane waves of the scattered electrons instead of plane waves, which considers the influence of hot dense plasma on the electron collision process. Finally, we study the electron-impact ionization process of Mg7+ in solid-density plasma using the theoretical model, which result in the increase of the ionization cross section by one order of magnitude compared with that of the isolated ion, And the result is an excellent agreement with the experimental result of Berg et al. The model shed some new insights on collisional ionization process, and would be used to study the radiation opacity and the nonequilibrium properties of hot dense plasma.

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Relaxation processes in dense plasmas

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Intensive studies of the properties of dense non-ideal plasma were triggered by the idea of realization of inertial confinement fusion. It should be noted that it is especially important to study relaxation times of electrons and ions. In particular, during compression of a target by the flow of high-energy electrons the non-isothermal plasma with heated electrons and cold ions is created [1-2]. Non-isothermal plasma also appears during interaction of heavy ion beams with a target [3]. In this work relaxation processes energy losses in dense plasma are obtained on the basis of the effective potentials [4-5]. A pseudopotential approach was used to study the effect of an ionic core on the electron-ion scattering in dense plasmas. Screening of the ion charge is taken into account using the density response function in the long wavelength limit. Additionally, the effect of electronic non-ideality is included using the compressibilty sum-rule connecting the local field correction and the exchange correlation part of the electronic free energy density [6]. The values of energy deposition, energy partition, temperature relaxation in a wide range of densities and temperatures for inertial confinement fusion applications have been calculated. The obtained results of relaxation processes in dense plasma are compared with the available experimental data and theoretical results of other authors [7].

This research was supported by the Ministry of Education and Science of Kazakhstan, under Grant AP08856650.

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Ultrafast Dynamics of Laser-Excited Topological Edge States in Graphene Nanoribbon Heterostructures

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The electromagnetic properties of finite graphene nanoribbon (GNR) heterostructures are strongly affected by localized topological edge states [1]. Recently, we showed for 7-9-armchair-GNRs that the increased electronic correlations of these states results in increased magnetic moments at the ribbon edges accompanied by a significant energy renormalization of the topological end states, even in the presence of a metallic substrate [2]. Here, we improve the description of the system by including long-range Coulomb interactions within the Pariser–Parr–Pople Model. Employing our newly developed DSL* approximation within the G1–G2 scheme we study the ultrafast electron response in a freestanding unit cell of the 7-9-armchair-GNR following a laser excitation. We find that the excited localized edge states play a major role in the subsequent electron dynamics.

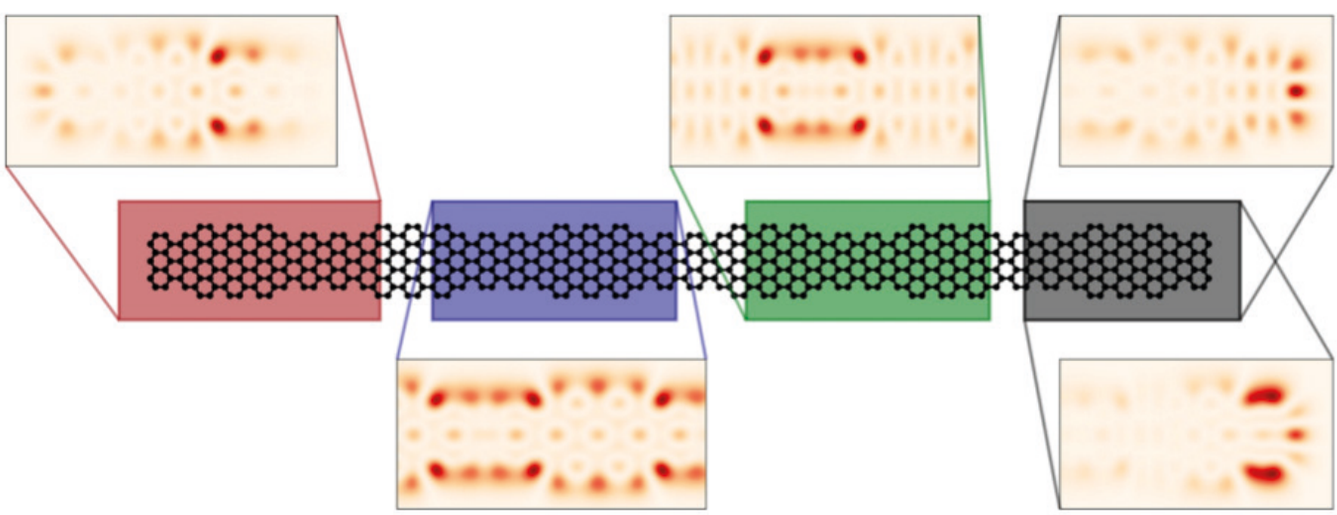

Figure 1: The GNR heterostructure (center) exhibits localized topological states depending on its shape and width. The local electron distribution corresponding to these topological states is visualized by the dark red areas in the boxes.

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A Kinetic Model of Friction in Strongly Coupled Strongly Magnetized Plasmas

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Plasmas that are strongly magnetized in the sense that the gyrofrequency exceeds the plasma frequency exhibit novel transport properties. Recent works studying the friction force acting on a massive test charge in a weakly coupled plasma have shown that strong magnetization leads to a transverse component perpendicular to both the Lorentz force and velocity of the test charge, in addition to the stopping power component that opposes the velocity. Molecular dynamics simulations have shown that strong Coulomb coupling in addition to strong magnetization gives rise to a third ``gyrofriction'' component in the direction of the Lorentz force. Here, we compute the friction force acting on a massive test charge moving through a strongly coupled and strongly magnetized one-component plasma using a generalized Boltzmann kinetic theory. The theory captures these effects and generally agrees well with the molecular dynamics simulations over a broad range of magnetization strength and Coulomb coupling regimes. Furthermore, either strong coupling or strong magnetization breaks a fundamental symmetry in traditional plasma theories: The friction force is dependent on the sign of colliding particles. This effect is known as the Barkas effect, and it reduces the stopping power and enhances the transverse and the gyrofriction components.

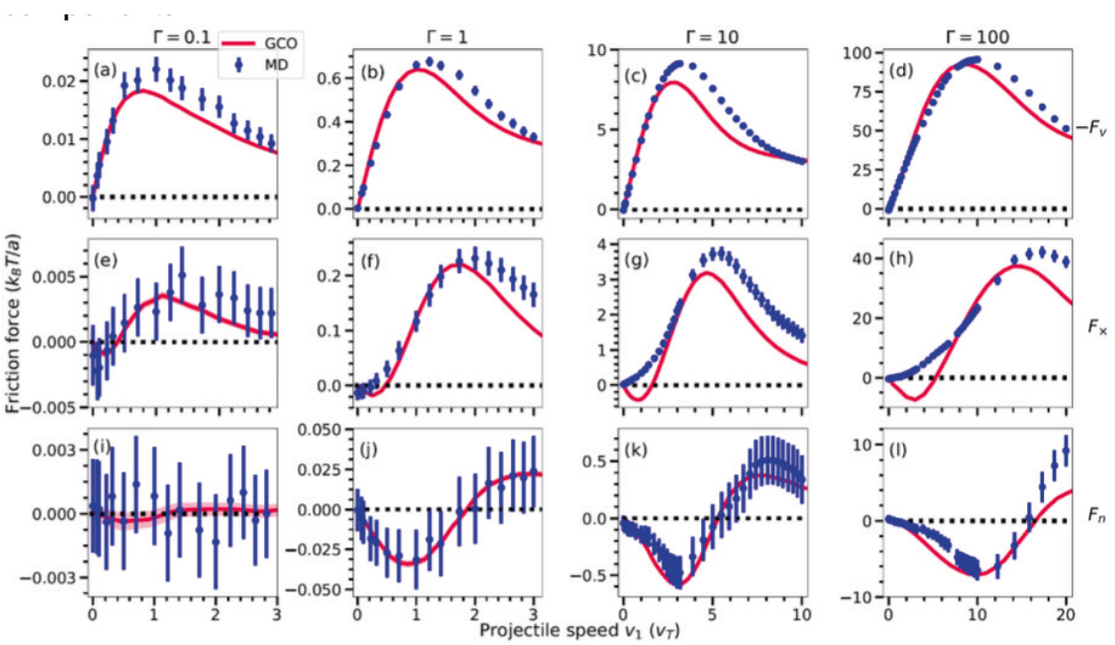

Figure 1: Comparison of the friction force computed using MD (red dots) and generalized kinetic theory (blue line) on a test charge moving through a strongly magnetized plasma for various coupling strengths. Figure from [1].

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Dynamic Structure Factor of the Magnetized One-Component Plasma: Crossover from Weak to Strong Coupling

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The dynamic structure factor (DSF) is of direct relevance for the analysis of x-ray Thomson scattering spectra. Here, we study the DSF of the classical one-component plasma under the influence of an external magnetic field with molecular dynamics simulations [1]. In particular, we investigate in detail the crossover from a weakly coupled to a strongly coupled state. While in weakly coupled plasmas the spectrum perpendicular to the field consists of a set of Bernstein modes [2], we observe higher harmonics of the upper hybrid mode in strongly coupled systems [3]. At moderate coupling strengths, the excitation of high-frequency modes is suppressed, and they can only be observed in strongly magnetized plasmas. Parallel to the magnetic field, the peak position of the plasmon is largely independent of the magnetization but its width increases, provided the plasma is strongly coupled.

Under oblique angles, two principal collective modes are found whose positions are in good agreement with cold-fluid theory. The dispersion of these modes strongly depends on the coupling and magnetization strengths. The simulation results are complemented by analytical theory for the DSF from the random-phase approximation, a Mermin-type dielectric function including collisions [4], and the quasi-localized charge approximation [5]. None of the theories can reproduce the transition that occurs when the system crosses the coupling regimes. The results are relevant to the scattering spectra and transport properties of dense magnetized plasmas.

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Electronic stopping in warm dense matter using Ehrenfest dynamics and time-dependent density functional theory

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Ehrenfest dynamics with time-dependent density functional theory (TDDFT) provides a framework for first-principles calculations of electronic stopping power that has been successfully applied in the solid state in numerous contexts. Its use in the warm dense regime has not been as widely studied, in part due to the computational expense of treating a large number of thermally occupied orbitals. In this talk, we examine some of the challenges associated with scaling Ehrenfest+TDDFT into the warm dense regime. We first consider isochorically heated aluminum, which allows us to study the impact of the pseudization of the L-shell under conditions in which it is increasingly thermally depleted. We then consider all-electron calculations of liquid-like deuterium and carbon to study the impact of finite-size effects and configurational averaging as a function of projectile energy. We conclude by taking the lessons we have learned to the analysis of electronic stopping in deuterium/beryllium mixtures relevant to fusion experiments. Throughout, we work within the context of validating average-atom models for the elemental systems and providing benchmark data for mixtures. We also report on some of the computational aspects of these calculations, which are among the largest of their kind.

SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

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Pressure effects on the electronic structure of carbon-hydrogen mixtures in the Mbar to Gbar regime

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High energy densities can significantly alter the electronic structure of materials. The pressure-induced insulator-metal transition of hydrogen is a model case that has been subject of theoretical and experimental studies for many decades. In the first part of the talk, I will present evidence for the creation of liquid metallic hydrogen in C-H mixtures shock-compressed to pressures around ~150 GPa and temperatures of ~5000 K, which was probed by different in situ X-ray methods at X-ray free electron lasers. Our observations suggest new ways to study the chemical properties of this exotic state in mixture with other elements, which is highly relevant for a better understanding for the interiors of giant planets. Moreover, exploting liquid metallic hydrogen chemistry may allow to realize the synthesis of highly interesting materials such as tailored nanodiamonds with specific color centers, new ultrahard forms of carbon or hydride-based compounds possibly providing room-temperature superconductivity.

At significantly higher pressures, i.e. approaching and exceeding the Gbar regime, partial pressure ionization of core electrons of light elements such as carbon is expected. Mimicking and probing such conditions in a controlled fashion is now possible at the National Ignition Facility. In the second part of the talk, I will summarize recent efforts to identify K-shell ionization of carbon in plasmas at conditions similar to the interiors of the smallest stars: so-called Red Dwarfs. Moreover, I will present first results of ongoing efforts to experimentally quantify radiation transport properties inside these highly interesting celestial objects.

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Transport evidence for a sliding two-dimensional quantum electron solid

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Ignited by the discovery of the metal-insulator transition [1], the behavior of low-disorder two- dimensional (2D) electron systems is currently the focus of a great deal of attention. In the strongly- interacting limit, electrons are expected to crystallize into a quantum Wigner crystal, but no definitive evidence for this effect has been obtained despite much experimental effort over the years. Here, studying the insulating state of a 2D electron system in silicon, we have found two-threshold voltage-current characteristics with a dramatic increase in noise between the two threshold voltages [2]. This behavior cannot be described within existing traditional models. On the other hand, it is strikingly similar to that observed for the collective depinning of the vortex lattice in Type-II superconductors [3]. Adapting the model used for vortexes to the case of an electron solid yields good agreement with our experimental results, favoring the quantum electron solid as the origin of the low-density state.

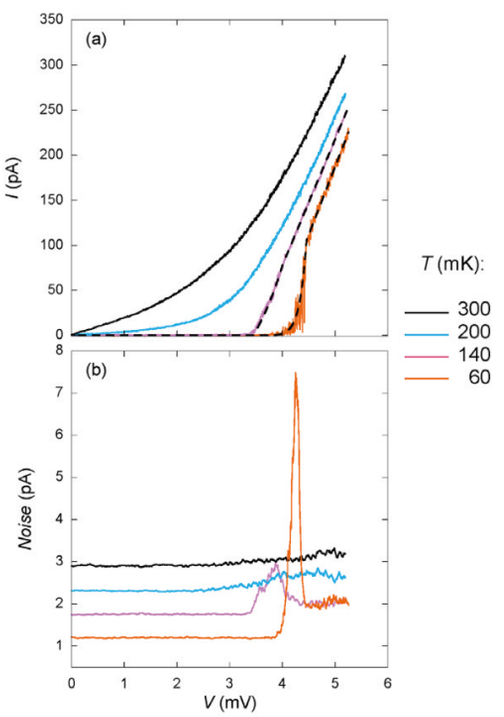

Figure 1: (a) Voltage-current characte- ristics at electron density ns=5.36x1010 cm-2 for different temperatures. (b) The broad-band noise as a function of voltage for the same electron density and temperatures. The three upper curves are shifted vertically for clarity.

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Quantum accurate interatomic potentials for warm dense matter

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Modeling warm dense matter is relevant for various applications including the interior of gas giants and exoplanets, inertial confinement fusion, and ablation of metals. Ongoing and upcoming experimental campaigns in photon sources around the globe rely on numerical simulations which are accurate on the level of electronic structures. In that regard, density functional theory molecular dynamics (DFT-MD) simulations [1] have been widely used to compute dynamical and thermodynamical properties of warm dense matter. However, two challenges impede further progress: (1) DFT-MD becomes computational infeasible with increasing temperature (2) finite-size effects render many computational observables inaccurate, because DFT-MD is limited to a few hundred atoms on current HPC platforms. Recently, molecular dynamics simulations using machine learning-based interatomic potentials (ML-IAP) could overcome these computational limitations. Here, we propose a method to construct ML-IAPs from DFT data based on SNAP descriptors [2]. We present our results for aluminum. In particular, we investigate the transferability of ML-IAPs over a large range of temperatures and pressures, which currently is a topic of active research.

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Dynamics of defect filaments in weakly disordered dust acoustic waves of dusty plasmas

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Dust acoustic wave (DAW), associated with the longitudinal oscillations of negatively charged micron-sized particles in gaseous plasmas, can be self-excited through the interplay of dust inertia, screened Coulomb interactions, and ion streaming. It is a paradigm for investigating and understanding of the generic behavior of nonlinear acoustic waves through directly tracking particle motion and waveform evolution over a large area [1-4]. In the weakly disordered state with waveform undulation of the single scale wave before the transition to wave turbulence, acoustic vortices with screw waveforms winding around fluctuating worm-like defect filaments can be spontaneously generated [1]. It leads to the name of defect mediated turbulence (DMT) for the single scale weakly disordered stated. Namely, those defect filaments can be viewed as singular objects for characterizing the waveform dynamics of the DMT state.

In this work, using the dusty acoustic wave generated in a radio frequency dusty plasma system, we experimentally investigate the dynamical behaviors of defect filament in the 2+1 dimensional spatio-temporal space of the DMT state by tracking the Lagrangian trajectories of defects. It is found that the temporal fluctuation of defect filament number exhibits a power spectrum with power law decay. A picture is constructed for explaining the observations of the Lagrangian dynamics, their attraction (repelling) under the same (opposite) topological charges, and their generation, traveling and annihilation under the deformed surrounding waveforms by their neighboring defects.

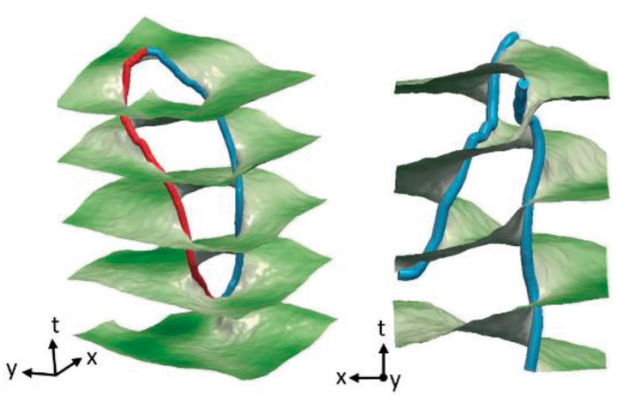

Figure 1: The plots of a pair of defect filaments with the opposite (same) topological charge and their surrounding stereo waveform of the wave crest surfaces. Positive and negative defects are colored by red and blue, respectively.

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Investigation of the stability of three-dimensional states of dynamic equilibrium of the two-component plasma of Vlasov-Poisson

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Set a definite formula:

$$\begin{gathered} f_t + \vec{v}\nabla_{\vec{x}} f - \nabla_{\vec{x}}\varphi\nabla_{\vec{v}} f = 0 \\ \Delta_{\vec{x}}\varphi = 4\pi(1 - \int\limits_{\Re^3} f(\vec{x},\vec{v},t))d\vec{v} \\ f = f(\vec{x},\vec{v},t) \geq 0; \quad f(\vec{x},\vec{v},0) = f_0(\vec{x},\vec{v}) \end{gathered} \qquad (1)$$

Which f – electron distribution function; t – time; $\vec{x}, \vec{v}$ – electron coordinates and speeds; φ –the potential of the self-consistent electric field; f_0 – initial data; f и φ – smooth function; the integral of the right side of the Poisson equation exists . Considering it is a sort of ions,which distribution function is isotropic and constant in physical space.
Derived a previously known sufficient condition for the linear stability of exact stationary solutions.

$$f = f^0(\vec{x},\vec{v}), \quad \varphi = \varphi^0(\vec{x}) \qquad (2)$$

the Vlasov-Poisson equations (1) with respect to three-dimensional perturbations:

$$\frac{df^0}{d\left(\frac{\vec{v}^2}{2}+\varphi^0\right)} \leq 0 \qquad (3)$$

Using hydrodynamic substitution of independent variables, the Vlasov-Poisson equations (1) are transformed to the previously known infinite system of three- dimensional equations similar to the equations of isentropic flow of a compressible fluid medium in the vortex shallow water and Boussinesq approximations.
By the direct Lyapunov method the absolute linear instability of exact stationary solutions (2) with respect to three-dimensional perturbations is proved. Thus, the sufficient condition of linear stability (3) is reversed and its formal character is revealed. An a priori exponential estimate of the growth of small three-dimensional perturbations from below is obtained.
The results of the present work are consistent with the well-known Irnshaw theorem on instability in electrostatics and extend its applicability from classical mechanics to statistical mechanics.

Research supervisor – Department of Physical and Mathematical Sciences. Associate Professor. Y.G.Gubarev

Charging of dust particles in the space

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Most of the space plasma is the so-called plasma with a condensed dispersed phase, i.e. the dusty plasma [1]. The study of dusty plasma under terrestrial conditions is of particular interest in connection with the possibility of the formation of ordered structures, direct observation of the dynamics of charged dust grains, and for a number of other important reasons. Dusty plasma particles under laboratory conditions are characterized by the Maxwellian distribution. However, studies of many works, including spacecraft data, have shown [2, 3] that in the solar wind, in the plasma of planetary magnetospheres, and in some other astrophysical objects, due to the presence of high-energy particles, there is a deviation from the equilibrium distribution of plasma particles. In most cases, the distribution has a power-law tail at high energies, corresponding to the κ (kappa) distribution.

In this work, we studied the process of charging dust particles within the kappa distribution. Using this distribution, expressions for the particle fluxes of the surrounding plasma to the surface of dust particles were obtained, and the equations of the OML (orbit motion limited theory) approximation describing the charging of dust particles were solved. The dependences of the dust particle's charge on the charging time, and also on other parameters such as the temperature ratio, etc. were obtained. An analysis of the effect of non-equilibrium distribution on charging, taking into account various charging mechanisms, was made. Finally, the computational software for studying the charging of dust particles has been developed on the Visual Studio 2019 platform.

This work was supported by the Grant AP09058005 of the Ministry of Education and Science of the Republic of Kazakhstan.

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Ab Initio Simulations for Warm Dense Matter with Applications in Planetary Physics

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Measurements by the Cassini and Juno spacecrafts have determined the gravity fields of Saturn and Jupiter with unprecedented precision. The interpretation of these measurements and the construction of interior models for these giant planets relies to a large degree on results from ab initio computer simulations of hydrogen, helium, and heavier elements at megabar pressures. Here we will review the uncertainties of the computed equations of state and identify conditions where the interior models are particularly sensitive to.
Then this talk will discuss recent findings of the Juno mission and explain why the unexpectedly low magnitudes of the gravity coefficients J4 and J6 imply that Jupiter has a dilute core at its center instead having of a traditional compact core that is composed to 100% of heavy elements.
For Saturn, this talk will discuss what we learned about the planet's prominent set of rings. Open questions about their mass, age, and origin will addressed.
This talk will conclude by sharing results from simulations of rock-ice mixtures for the interior of water worlds. It will be determined what pressure-temperature conditions are needed for rocky and icy materials to become miscible in all proportions and when they can be reached during the formation of a planet.

Direct imaging of phase transitions in nonequilibrium warm dense matter

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Intense optical irradiation can bring matter into highly non-equilibrium warm dense states. Understanding the structural properties of these transient states is important for many applications including laser micromachining, planetary sciences, and inertial confinement fusion experiments. However, direct observation of phase transitions under warm dense matter (WDM) conditions has been challenging because of the ultrasmall length scales and ultrafast time scales involved with the dynamic processes. Recent development of MeV ultrafast-electron diffraction (MeV-UED) enables to follow dynamics with Ångstrom spatial and femtosecond temporal resolution, making it a perfect tool to study phase transitions under these extreme conditions.
In this talk, I will present our recent work using single-shot MeV-UED [1] to study phase transitions and structural dynamics in nonequilibrium WDM created by ultrafast laser excitation of solids and liquids. The talk will be focused on the following applications: mapping ultrafast melting process in warm dense gold [2], visualizing ultrafast melting initiated by radiation-induced defects [3], and imaging the structural evolution in strongly excited liquid water.

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Analyzing XC functionals for electronic structure calculations at WDM parameters

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In this presentation we discuss the results of the analysis of the accuracy of the commonly used exchange-correlation (XC) functionals for warm dense matter simulations [1,2]. The analysis is performed by comparing highly accurate path-integral quantum Monte-Carlo (QMC) data with KS- DFT results. The relative deviation of the total density from the reference data is reported for different XC functionals in the case of the inhomogeneous electron gas. Furthermore, a new methodology for the investigation of the non-linear static density response WDM based on the KS-DFT method is presented [3]. The results are verified by comparing to the QMC data when the thermal temperature is equal to the Fermi temperature. New results for partially and strongly degenerate electrons are presented. Finally, we present the results of the analysis of the electronic local field correction as computed using various XC functionals. By comparing the data to the exact QMC results, we are able to understand the effect of thermal excitations on the XC functional.

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Itinerant-electron magnetism: the importance of many-body correlations

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Do electrons become ferromagnetic just because of their repulsive Coulomb interaction? Our calculations on the three-dimensional electron gas imply that itinerant ferromagnetim of delocalized electrons without lattice and band structure, the most basic model considered by Stoner, is suppressed due to many-body correlations as speculated already by Wigner, and a possible ferromagnetic transition lowering the density is precluded by the formation of the Wigner crystal.

Molecular dynamics modeling for studying the effects of dusty plasma in cryogenic conditions

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The velocity autocorrelation function was calculated using the 3D Molecular dynamics method. In this simulation number of particles was taken as 27000. Calculations were done by taking into consideration neutral shadowing force to evaluate the impact on the VAF [1]. In Figure 1, at rcut =1 no force effect was observed regardless of plasma parameters such as Γ, k, [2]. On the contrary, in the case when rcut =2, the neutral shadowing force has a significant effect on the VAF with an increase in the value of . The neutral force at rcut =2 affects the stronger manifestation of transverse waves [3].

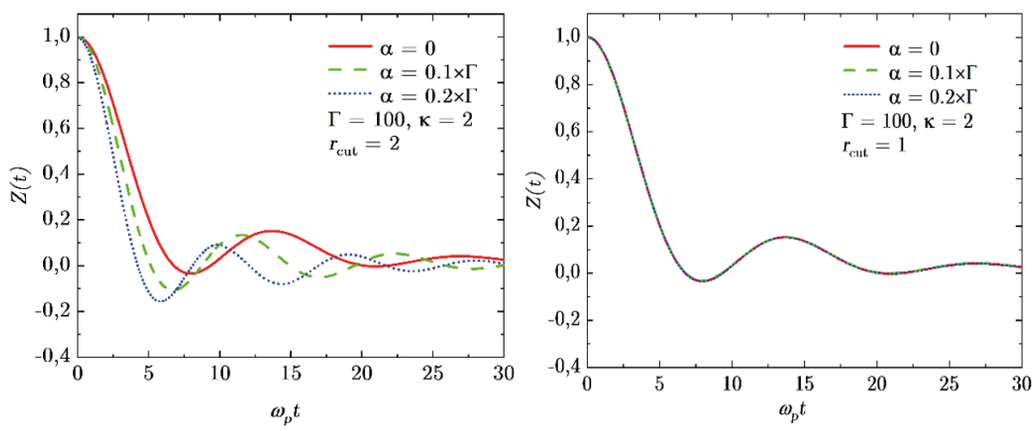

Figure 1: Velocity auto-correlation function at Γ = 100, rcut =1 and , rcut =2.

Using the next function, the spectrum of the velocity autocorrelation function was calculated :

$$Z(\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} Z(t)\exp(i\omega t)dt,$$

where Z(t) is VAF.

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Coulomb effects in electronic transport

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Conventional experiments aimed at uncovering inner workings of solids often rely on transport measurements, the tool that proved to be indispensable throughout the history of condensed matter physics. In a traditional experiment one measures a current-voltage characteristic and extracts linear response functions determined by properties of the unperturbed system. A basic quantity that can be measured in this way is the Ohmic resistance R. The traditional approach has been very successful in experimental studies of low-temperature properties of conventional conductors, where the observable behavior of the electronic system is largely governed by a single scattering mechanism due to potential disorder, while the role of electron-electron interaction is limited to small corrections [1]. In contrast, properties of strongly correlated systems, or more generally, any many body systems where quasiparticle (Coulomb) interactions are at least as important as one-particle scattering processes are much harder to establish experimentally and to describe theoretically. In this talk I will give a brief overview of physical phenomena arising solely due to Coulomb interaction between electrons (more generally, charge carriers) including Coulomb drag [2] and signatures of collective (hydrodynamic) flows of charge and energy [3,4].

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Deep Quantum Monte Carlo

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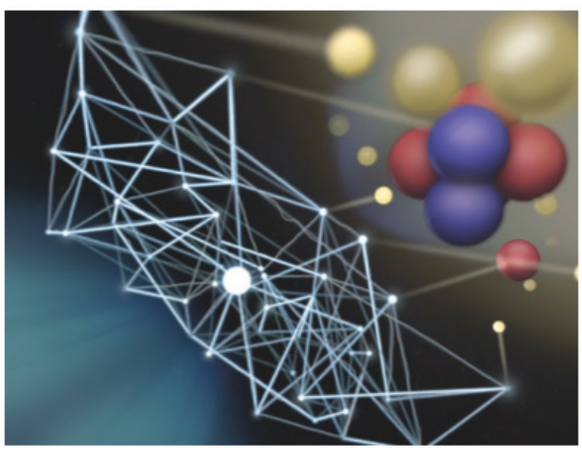
Deep learning has had profound impact on various technologies and is now also increasingly used in scientific discovery. One of the fundamental outstanding problems of Physics and Chemistry is the electronic structure problem, i.e. the accurate solution of quantum states of the electronic many-body Schrödinger equation.
Following Carleo and Troyer's approach of solving neural network states for Bosonic lattices we have developed PauliNet [1,2], a deep neural network for representing fermionic states that incorporates the Physics of electronic wavefunctions and is trained by variational Monte Carlo. PauliNet achieves high-accuracy solutions to the electronic ground-states given only the Hamiltonian as an input and with relatively low computational complexity. We have also extended this approach to compute excited states [3]. I will give an overview of the technology and describe recent developments.



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The study of temperature relaxation in dense plasma by the method of molecular dynamics

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Currently, active studies of the properties of dense non-ideal plasma are being conducted in connection with the problem of the implementation of inertial thermonuclear fusion. It should be noted that the study of the relaxation processes of the temperatures of electrons and ions is particularly relevant in order to verify modeling methods.

In the present work, we apply the molecular dynamics method to simulate temperature relaxation for dense plasma. The problem of temperature relaxation has been discussed by many authors, beginning with the first kinetic models, as well as by methods of computational experiment [1–2]. For high-temperature plasma of inertial thermonuclear fusion, the Coulomb potential is a good model for the interaction potential. The system must be supplemented with boundary conditions. For this setting, various boundary conditions are possible, most often periodic or mirror boundary conditions are used. With temporary relaxation of the initial state, the temperatures equalize. Plasma can be trapped or fly apart into a vacuum - in any case, the interaction of the electronic and ionic subsystems leads to the equalization of temperatures.

The classical problem of energy relaxation in a plasma of positronium, hydrogen and helium is considered. The results on the equalization of electron and ionic temperatures at different mass ratios are obtained, the relaxation times of temperatures are determined. The results of the calculations are the dependences of the kinetic energy of the electronic and ionic subsystems as a function of time. To show the correctness of the model, its results are compared with the results of available results of simulations.

This research was supported by the Ministry of Education and Science of Kazakhstan, under Grant AP09258792.

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Josephson effect and superfluidity in electron-hole bilayer heterostructures

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We analyze the superfluid characteristics and crossover physics for Josephson junctions [1] in electron-hole bilayer TMD semiconductors [2]. We determine the critical current across junctions of different potential barrier heights [3,4]. We show that the crossover physics in the narrow barrier region controls the critical current throughout. We find that the ratio of the critical current divided by the carrier density exhibits an observable maximum at the density of the switchover from bosonic excitations to pair-breaking fermionic excitations. This provides, for the first time in a semiconductor system, an experimental measure for the position of the boundary separating the BEC and BCS-BEC crossover regimes.

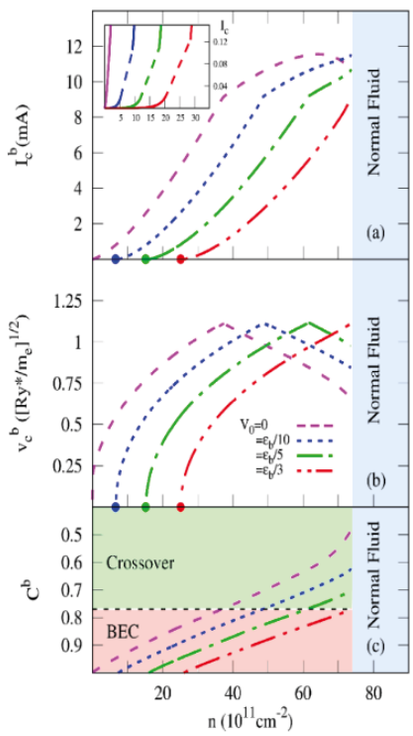

Figure 1: Critical current (a), critical velocity (b), condensate fraction (c) for different barrier heights V0.

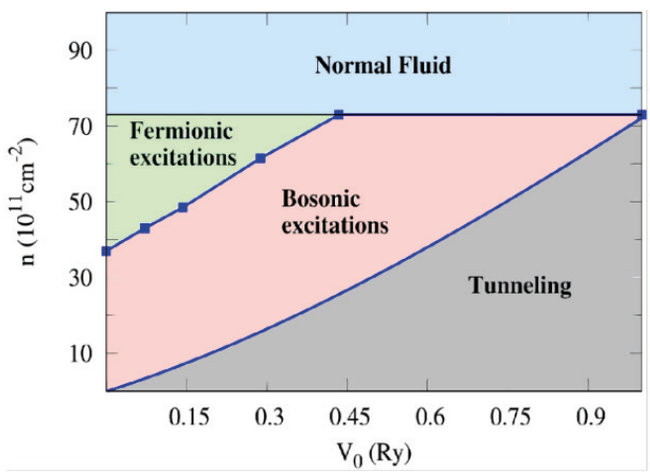

Figure 2: Critical current driving mechanisms.

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High-Tc electron-hole superfluidity and BCS-BEC crossover in double-layer heterostructures

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In recent years there have been a growing theoretical and experimental interest in double electron-hole layers. These Coulomb systems include GaAs double quantum wells (DQW) [1] and, more recently, double graphene bilayers (DBLG) [2], double transition metal dichalcogenides (DTMD) [3], and Ge-Si heterostructures [4]. A key motivation for the studies has been that a direct Coulomb attraction generates strongly bound electron-hole pairs in these solids and large superfluid gaps that are able to suppress the detrimental Coulomb screening in a self-consistent way. The electron- hole pairs may condense into a superfluid/BEC at low enough temperatures, and there is now experimental evidence that this indeed happens. I will discuss the efforts done in these systems to maximise the strength of the electron-hole pairing with the aim to increase the critical temperature for superfluidity and the superfluid gaps [5,6].

Increasing the density of electrons and holes, the superfluid BEC-BCS crossover can be induced and tuned in these systems. We investigate the BEC-BCS crossover phenomena using a comprehensive mean-field multicomponent model. We determine the momentum dependent multicomponent superfluid gaps, the corresponding condensate fractions, and the chemical potential. The pairing interaction is Coulomb long-ranged and self-consistently screened.

In the case of DBLG and DTMD, we demonstrate the superfluidity in these systems is dominated by multicomponent condensates with strikingly different properties. We found that the origins of multicomponent superfluidity in DBLG and DTMD systems are fundamentally different. In graphene, superfluidity is multicomponent because of the small tunable bandgap between the conduction and valence bands, while in DTMD it is multicomponent because of the splitting of the bands caused by the strong spin- orbit coupling. Interestingly, the multicomponent nature of the superfluidity can be switched on and off, in the case of DBLG by tuning the bandgap, and in the case of DTMD by tuning the density and switching the doping. We determine optimal ranges of densities for maximising the Tc of the superfluidity for these two systems.

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Collective excitations in beyond-graphene atomically thin materials

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Experimental probes that access the response of strongly interacting electron liquids at finite in-plane momentum q and frequency ω are expected to be rich sources of information. One of these probes is scattering near-field optical microscopy (SNOM), which enables the measurement of the dispersion relation of collective electronic excitations, such as Dirac plasmons in graphene. In this talk, I will discuss how SNOM can unveil the collective plasmonic modes of electrons roaming in twisted bilayer graphene [1] and present a theoretical approach [2] to calculate their spectra. I will try to argue that near-field optical probes offer new insights, complementary to those offered by other techniques, on the carrier dynamics in this correlated electron system. If time allows, I will also present a recent theoretical approach [3] to calculate the dispersion relation of plasmon-magnon collective modes in two-dimensional honeycomb magnets.

Work supported by the European Union's Horizon 2020 research and innovation programme under grant agreement No. 881603 "GrapheneCore3".

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Material properties of matter in Saturn's interior from ab initio simulations

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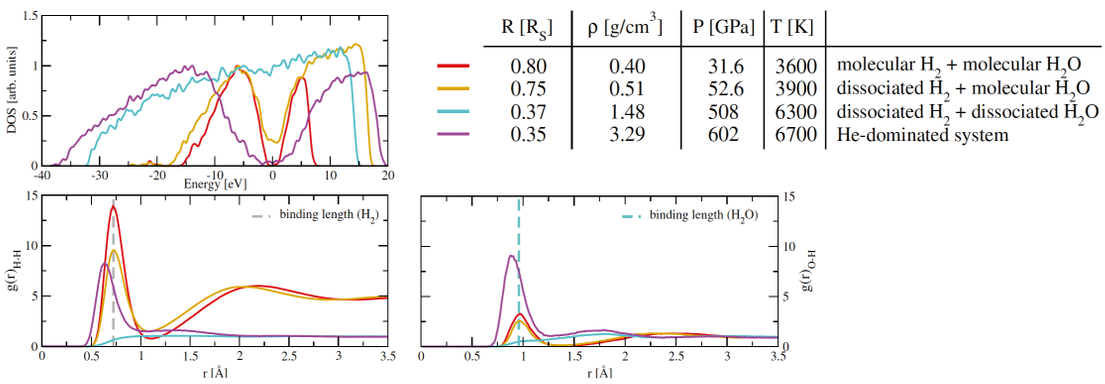
Calculation of material properties from ab inito simulations along Jupiter [1] and Brown Dwarf adiabats [2] have been subject of earlier studies. However, accurate models of Saturn's interior are still very challenging. A recent study by Mankovich and Fortney on Jupiter and Saturn models was based on a single physical model [3] which predicts a strongly differentiated helium distribution in Saturn's deep interior, resulting in a helium-rich shell above a diffuse core.



R [R_S]	ρ [g/cm^3]	P [GPa]	T [K]	
0.80	0.40	31.6	3600	molecular H_2 + molecular H_2O
0.75	0.51	52.6	3900	dissociated H_2 + molecular H_2O
0.37	1.48	508	6300	dissociated H_2 + dissociated H_2O
0.35	3.29	602	6700	He-dominated system

Figure 1: The DOS (upper left) and the pair distribution function of H-H (lower left) and O-H (lower right) at dedicated points of interest (upper right).

We focus on the calculation of material properties of matter at P-T conditions along the Saturn model proposed by Mankovich and Fortney. The dissociation of hydrogen as well as the onset of the helium-rich layer have profound impact on material properties: Dissociation of hydrogen triggers the metallization of the hydrogen subsystem and the band gap of the system closes. However, helium is still an insulator under all the conditions of the model [4,5]. The onset of the helium-rich layer in the deep interior therefore again changes the properties of the mixture: Molecular hydrogen dominates the outer atmosphere, followed by a layer of mainly metallic hydrogen in the interior, followed again by a layer of helium-dominated insulating material above the core. We present results on thermodynamic and transport properties of a hydrogen-helium-water mixture that closely resembles the element distribution of the Saturn model. We discuss implications of the results on our understanding of Saturn's interior and evolution.

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Electrical Conductivity of Iron in Earth's Core from Microscopic Ohm's Law

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Understanding the electronic transport properties of iron under high temperatures and pressures is essential for constraining geophysical processes. The difficulty of measuring the electrical conductivity of iron under Earth-core conditions reliably in experiments [1] calls for sophisticated theoretical methods that can support diagnostics. We present results of the electrical conductivity in iron within the pressure and temperature ranges found in Earth's core from simulating microscopic Ohm's law using time-dependent density functional theory. Our predictions [2] provide a new perspective on resolving discrepancies in recent experiments [3,4].

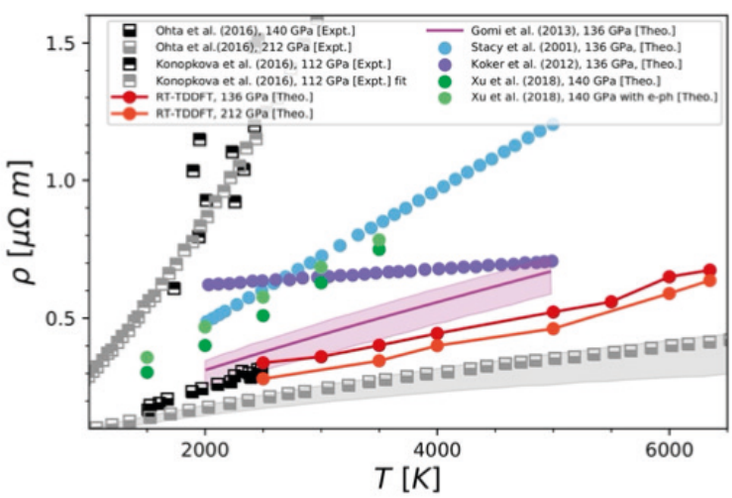

Figure 1: Electrical resistivity and its temperature dependence at fixed, high pressures.

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Ion core effect on transport and thermodynamic properties in dense plasmas

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Dense plasmas are generated in modern high-energy-density-plasma science facilities such as NIF, GSI, Sandia National Laboratory, where the dense plasmas are created by compressing and heating a target by a laser or intense charged particle beams. In this work, we present the results of calculations of the transport and thermodynamic properties of dense plasma at ICF parameters. It is known that the interaction potentials between particles are also of importance for correctly calculation of plasma properties taking into account peculiarities and parameters of investigated plasma [1]. Transport and thermodynamic properties are studied on the basis of screened electron-ion interaction potentials [2-5]. A pseudopotential approach was used to study the effect of an ionic core on the electron-ion scattering in dense plasmas. Screening of the ion charge is taken into account using the density response function in the long wavelength limit. Additionally, the effect of electronic non-ideality is included using the compressibility sum-rule connecting the local field correction and the exchange correlation part of the electronic free energy density. Using screened effective potential, we have computed electron-ion scattering phase shifts, the total elastic scattering cross section, and the transport cross section. It is found that the ionic core leads to the strong decrease of the scattering cross sections, transport and thermodynamic properties. Additionally, it is shown that the transport cross section has a non-monotonic dependence on the variation of the ionic core field parameters. To show the correctness of the model, its results are compared with the results of MD and QMD simulations [6].

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Thermodynamic and transport properties of plasmas: numerical simulations and benchmarks from analytical theory

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The properties of plasmas are expressed in terms of correlation functions, which can be evaluated using different approaches (analytical theory, numerical simulations).

Analytical expressions obtained from perturbation theory (method of Green's functions) are approximations, but provide benchmarks, e.g. for the low-density limit. Expansions with respect to density (virial expansions) are considered for different thermodynamic and transport properties.

Numerical results for the electrical conductivity of hydrogen plasmas are obtained from molecular dynamics simulations based on density functional theory (DFT-MD) in the low-density and high-temperature regime and compared with virial expansions [1]. The account of electron-electron collisions is discussed. We have found that the evaluation of the Kubo-Greenwood formula using DFT-MD simulations does not include the electron-electron scattering effects (such as the Lorentz plasma model) and cannot reproduce the low-density limit of the electrical conductivity of hydrogen plasmas.

Another numerical approach, the path-integral Monte Carlo (PIMC) simulations, is able to account for the effects of electron-electron scattering. Calculations of the electrical conductivity of hydrogen plasmas would be of interest, but have not yet been performed. PIMC simulations have been successfully used to calculate the thermodynamic properties of the uniform electron gas. Comparison with higher-order virial expansions that serve as benchmarks is possible. In particular, we show that high-precision PIMC simulations confirm the correct form of virial expansion, which has been debated recently.

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Doublon production in correlated materials by multiple ion impacts

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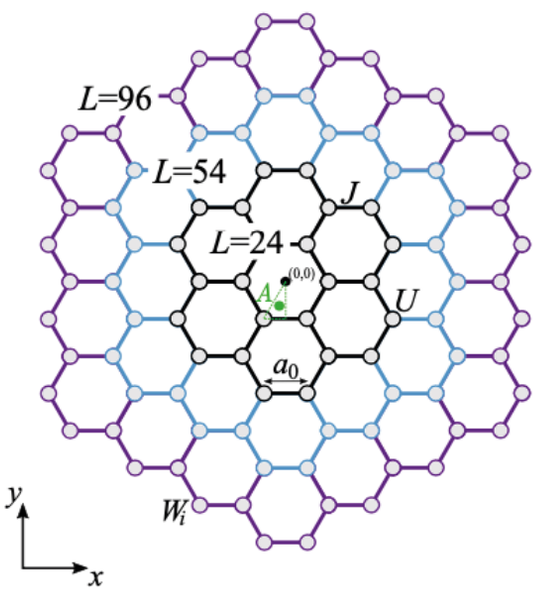
In a recent Letter [1] it was demonstrated that ions impacting a correlated graphene cluster can excite strong nonequilibrium states. In particular, this can lead to an enhanced population of bound pairs of electrons with opposite spin—doublons— where the doublon number can be increased via multiple ion impacts. These predictions were made based on nonequilibrium Green functions (NEGF) simulations allowing for a time-dependent non-perturbative study of the energy loss of charged particles penetrating a strongly correlated system.
In my talk, I will present recent results [2] where we extended these simulations to larger clusters and longer simulation times, utilizing the recently developed G1–G2 scheme [3] which allows for a dramatic speedup of NEGF simulations. With this improved accessibility, we were able to perform systematic analyses of the dynamics and to investigate the dependence of the energy and doublon number on the time interval between ion impacts and on the impact point.



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Ab initio simulations for the ion-ion structure factor of warm dense aluminum

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We calculate the intermediate scattering function of warm dense aluminum by using density functional theory molecular dynamics simulations. From this data set we derive the static and dynamic ion-ion structure factors. By applying a generalized collective modes model, we can fit the excitation spectra of the ion system and thereby extract the dispersion for the ion acoustic modes, as well as the decay coefficients for the diffusive and collective modes. The results are discussed and compared with experimental data if available. We show that computational limitations prevent sufficient access to the hydrodynamic limit and demonstrate that this can be circumvented using high-dimensional neural network potentials. We extract the ionic thermal conductivity of aluminum in the hydrodynamic limit and compare it to values computed using a Green-Kubo relation. We highlight the importance of partitioning the heat capacity into electronic and ionic contribution and only using the ionic contribution to compute the thermal conductivity of the ions in the hydrodynamic limit.

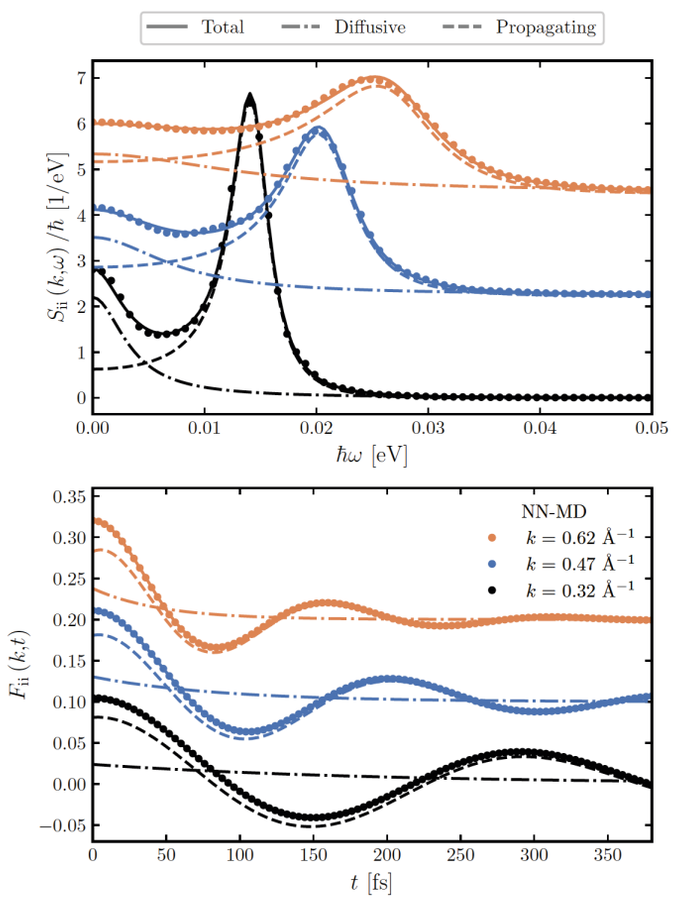

Figure 1: The dynamic ion-ion structure factor (upper panel) and the intermediate scattering function (lower panel) of warm dense Aluminum at T=1eV and ambient density, computed from DFT-MD simulations are shown. The fits to the diffusive and propagating modes are indicated by dash-dotted and dashed lines, respectively.

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Electron capture in the degenerate partially ionized plasmas

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To solve the actual problems of thermonuclear controlled fusion (TCF) with inertial confinement [1], as well as to study the processes taking place in astrophysical objects (white dwarfs, the Sun, the bowels of giant planets, etc.), reliable data on the physical characteristics of a nonideal degenerate plasma arising on Earth and in the Cosmos in many processes associated with the heating and compression of matter are needed.

Recombination can take place at the collision of an electron with an ion if the latter capture the electron. The process of electron capture by an atom has been investigated in many studies [2–3]. A neutral hydrogen atom can be converted to a negative hydrogen ion because of the polarization capture of the electron. In [4] the electron capture cross section was theoretically considered, and a method for finding the capture radius based on perturbation theory was used. To find the capture radius, capture time, and probability of electron capture, the Bohr–Lindhard method [3–4] was applied. The influence of the electron–exchange and plasma was discussed in the Ref. [5]. The influence of the nonthermal screening on the formation of the negative hydrogen ion in partially ionized generalized Lorentzian plasmas was investigated in [2].

In this work, the process of electron capture in nonideal dense plasma with degenerate electrons has been investigated. For this goal the Bohr–Lindhard method has been applied to obtain the electron capture cross section. All calculations have been done in the framework of the trajectories of incident electron near hydrogen ion (proton) obtained by the numerical simulation of the equations of motion. The effective interaction potential [6-7], which takes into account the screening effects at large distances and effects of the quantum non-locality, was used. The results of numerical calculations of the electron capture radius, differential and total cross section for different values of the density parameter and energy are presented.

The authors acknowledge support from the Science Committee of the Ministry of Education and Science of the Republic of Kazakhstan under Grant No. AP13067741.

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Debye plasma model under scrutiny: Rydberg excitons as testing probes for low-density electron-hole plasmas

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It is a persistent myth in plasma physics that the Debye-Hückel theory provides an appropriate description of low-density plasmas, even though theoretical investigations have cast considerable doubt on this assumption [1]. One main reason could be the lack of a decisive experimental test, since the measurement of the plasma-induced shift of single-particle energies in atomic systems is notoriously problematic.

Remedy can be found in solid-state systems, more precisely in Rydberg excitons, i.e. electron-hole bound states with a high principal quantum number [2]. These objects turn out to be highly sensitive probes for their surrounding making it possible to unravel accurately the basic properties of low-density nondegenerate electron- hole plasmas [3].

We analyze recently measured absorption spectra of bulk cuprous oxide crystals in which a tailored electron-hole plasma has been generated optically [4]. Special attention is paid to energies and linewidths of Rydberg excitons as well as to the position of the band edge. These quantities are compared to theoretical predictions. Our analysis confirms previous theoretical findings by demonstrating unambiguously that the plasma impact on the bound states cannot be described by the classical Debye model, but requires a quantum many-body theory. We discuss whether this result is of general validity.

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Collective excitations and quantum incompressibility in electron-hole fluids

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We have recently extended to electron-hole bilayers [1] the quantum continuum mechanics (QCM) formalism [2], which expresses excitation energies at T = 0 in terms of ground-state pair correlation functions and kinetic energy. The final formulas for the collective modes deduced from this approach coincide with the formulas obtained in the QLC approximation of Kalman and co-workers, as adapted to e-e bilayers [3], once the non-interacting kinetic energy is replaced with the interacting one. In the charged channell the theory [1] predicts the existence of gapped excitations, with the gap arising from electron-hole correlation, with the consequence that the static density-density response function vanishes as q2 for q → 0, rather than linearly in q, as commonly expected, pointing to an incompressibility of the system. This feature, which has no analog in the classical electron-hole plasma, is consistent with the existence of an excitonic ground state and implies the existence of a discontinuity in the chemical potential of electrons and holes when the numbers of electrons and holes are equal. It should be experimentally observable by monitoring the densities of electrons and holes in response to potentials that attempt to change these densities in opposite directions. I will first briefly review our findings for the electron-hole bilayers when using structure and kinetic energy from (i) accurate DMC simulations [4] or (ii) a BCS selfconsistent scheme. I will then turn to the application of the QCM to a 3-dimensional electron-hole homogeneous fluid at T = 0, stressing similarities and differences with the 2-dimensional counterpart. I will then present preliminary numerical results obtained using ground-state structure and kinetic energy computed within a BCS selfconsistent scheme.

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Physics-Informed Neural Networks for Quantum Dynamics of Electrons

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Time-dependent density functional theory (TDDFT) is an important method for simulating dynamical processes in quantum many-body systems. We explore the feasibility of physics-informed neural networks as a surrogate for TDDFT. We examine the computational efficiency and convergence behaviour of these solvers compared to state-of-the-art numerical techniques on models and small molecular systems. The method developed here has the potential to accelerate the TDDFT workflow, enabling the simulation of large-scale calculations of electron dynamics in matter exposed to strong electromagnetic fields, high temperatures, and pressures.

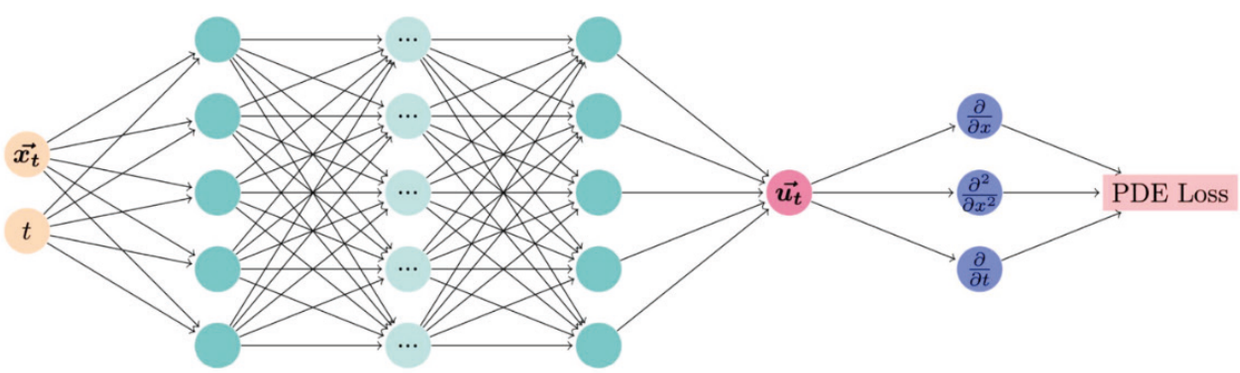

Figure 1: Architecture of Physics-Informed Neural Networks

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Inelastic collisions in the dense partially ionized plasmas

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The study of bound states in dense plasma has always been of great scientific interest. It is known that the plasma environment leads to screening of the charge's field not only in free states but also in the bound states. In particular, this leads to broadening and shift of the spectral lines [1-2]. Also, due to the screening effect, as well as the energy level broadening in the external plasma microfield, the upper energy levels cease to exist. This trend intensifies with increasing plasma density. Thus, when a certain critical density value is reached, a sharp increase in electrical conductivity occurs. This is connected, as already noted, with the disappearance of bound states (pressure ionization). Mott was the first, who connected this phenomenon with the screening of the Coulomb interaction, therefore it was called the Mott transition [3-6]. The Mott effect is taken into account to determine the dense plasma composition, for example, by solving the Saha equation with introduction of the lowering of the ionization potential. The correction to the ionization potential depends on the screening effect.

In this work, the interaction potential [7] of dense plasma particles, which takes into account the effect of quantum non-locality as well as electronic correlations, was used to solve the Schrödinger equation for the hydrogen atom. Energies of bound states and wave functions of the hydrogen atom were calculated. The results obtained are in good agreement with the results of other authors. Then, using these data, the cross sections for the excitation of a hydrogen atom by electron impact were calculated.

The authors acknowledge support from the Science Committee of the Ministry of Education and Science of the Republic of Kazakhstan under Grant No. AP13067741.

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How 2D solid loses its structural order in the KTHNY melting transition through defect excitation

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It is widely accepted that the melting transition governed by the Kosterlitz-Thouless- Halperin-Nelson-Young theory [1,2,3] is a two-stage transition through the intermediate hexatic phase. The pair generation and separation of dislocation defects have been demonstrated as the causes for the loss of translational order by various numerical simulations [4]. However, the spatiotemporal behaviors of topological defects in the solid close to the hexatic phase still remain elusive. Here, this issue is numerically addressed by using a 2D Yukawa system heated to nearby the hexatic point. It is found that the thermally excited collective particle motions cause lattice wiggling and distortion, which in turn generate dislocation defects through bond breaking/reconnection. The successive generation, traveling, interaction, annihilation of dislocation defects under the conservation of Burgers vector, can lead to the intermittent emerging of local crystalline ordered domains with different lattice orientations, surrounded by dislocation defect strings.

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Exchange effects in plasmon dispersion

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The Quasi-Localized Charge Approximation developed by Kalman and Golden in the 1990's [1] was aimed at describing the collective behavior of charged particle many body systems in the strongly coupled liquid state. Its application to a variety of such systems has been able to predict significant features of collective behavior. The QLCA is based on the simple physical idea that in the strongly coupled phase the particles get localized in randomly distributed but correlated temporary potential traps and it is the coupled dynamics of the localized oscillations of the particles in the traps that appear as collective excitations. While the above picture is an inherently classical one, there is little doubt that the same physics applies to a degenerate electron liquid. At the same time, significant differences arise between classical and quantum systems that are both of substance and of formalism. The main new effect that enters the mechanism of generation of collective modes stems from the required anti- symmetrization of the localized wave functions. The proper inclusion of the resulting "exchange interaction'' in the determination of equilibrium properties of solids has been a central theme in condensed matter physics since the early days of quantum theory [2].

Here we attempt to explore the dynamical consequences of the "exchange interaction". We do this by focusing on a pair of neighboring electrons trapped in their respective potential traps and calculate their ground state singlet and triplet energies. Then we argue that the second derivative of the energy expression with respect of the separation distance between the traps may be regarded as an effective potential. This effective potential is entered as pairwise interaction in the QLCA formalism in order to calculate plasmon and related dispersion relations. We use the Heitler-London approximation to calculate the exchange potential for two different trap models, obtaining a good qualitative agreement between them. In the resulting dispersion relation caused modifications of the classical results show up mostly at high k-values, not surprisingly, since exchange is a short-range effect. There is no modification over the classical result at k=0.

The approach described here has a few obvious flaws as far as the simple superposition of binary exchange are concerned. We point out possible directions to improve upon this aspect of the theory in future works.

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Low frequency second plasmon in an electron liquid

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Through the application of the newly established exchange augmented Quasi- Localized Charge Approximation [1] we establish the existence of a new low frequency "second plasmon" in a strongly coupled electron liquid. From its dispersion and its satisfaction of the 3rd frequency sum rule we identify it as the strong coupling manifestation of the elusive magnetic excitation conjectured earlier for an electron gas [2].
It is basically a two-component effect maintained by the short-range antiferromagnetic correlations in the electron liquid, governed solely by the Coulomb interaction between the spin-up and spin-down densities. Concerning its characteristic frequency, $\omega 2$ is proportional to the $r = 0$ value of the spin-up/spin-down correlation function. The spectral weight of the excitation is manifest in the partial spin-resolved dynamical structure functions. An independent derivation based on a generalized Feynman Ansatz corroborates this result. The relationship to the recently identified [3] "spin plasmon" excitation is discussed. Scattering experiment with polarized neutrons or polarized X-rays may provide a possible avenue to observe equilibrium fluctuations associated with this mode.

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Sarkas: A Fast Pure-Python Molecular Dynamics Suite for Non-Ideal Plasmas

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Molecular Dynamics (MD) is a powerful tool for simulating complex dynamical systems. MD is used across several disciplines and their sub-fields, e.g. biology, chemistry, material science. In fact, for each of these research fields we can find MD codes, open-source or proprietary, optimized for the simulation of their respective dynamical systems. No such code exists for Non-Ideal Plasmas. This generates several difficulties for researchers. On one hand researchers are forced to modify existing codes and/or write their own. This requires an extensive knowledge of computing as all the available codes have been developed in low-level languages, e.g. C or Fortran. Furthermore, the codes have been optimized for the simulation of systems other than non-ideal plasmas and as such are often difficult to modify. On the other hand, most MD codes provide only a code for the simulation phase and lack pre- processing and/or post-processing analysis tools. Several open-source packages are available for post-processing, but again they are specific to systems other than non- ideal plasmas and are often developed in interpretative languages, e.g. Python. Here we present Sarkas: a fast pure-python MD suite for non-ideal plasmas. Sarkas aims at lowering the entry barrier for computational plasma physics by providing a comprehensive MD suite complete of pre- and post-processing tools most common in plasma physics. It offers the ease of use of Python while being highly performant with execution speeds comparable to that of compiled languages. Its high-performance originates from the extensive use of NumPy arrays and Numba's just-in-time compilation. Sarkas is built in a modular fashion to allow easy implementation of additional features. It offers a variety of interaction potentials commonly used in plasma physics, Coulomb, Yukawa, Quantum Statistical Potentials. Furthermore, Sarkas' built-in pre-processing and post-processing libraries for data analysis allow researchers to get publication-grade results in less time [1-2].

Work supported by a US AFOSR Grant No. FA9550–17-1–039. U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52- 07NA27344
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Temperature relaxation in strongly-coupled binary ionic mixtures

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Relaxation in non-ideal plasmas is a complex process that involves expansions/contractions, thermal conduction, thermalization and temperature equilibration. Unfortunately, very little is known experimentally about these processes because of the challenges associated with isolating them individually. As such, we rely heavily on unvalidated theoretical models. This knowledge gap is particularly large for the very challenging case of ionic relaxation. Current improvements in experimental techniques now allow for the creation of ultracold binary mixtures for the investigation of equilibrium relaxation phenomena dominated by ion-ion collisions. These experiments, when complemented by large-scale molecular dynamics (MD) simulations, promise to provide detailed data on these processes. We have modeled a binary relaxing ultracold neutral plasma with MD, motivated by experiments at Brigham Young University, and compared the results to the most common theoretical models. None of the temperature relaxation rates from current theoretical models is within an order of magnitude of the MD simulations, suggesting serious gaps in our knowledge of ionic relaxation. We argue that such disagreement is due to dynamical correlations neglected by the currently available theoretical models [1,2].

Work supported by a US AFOSR Grant No. FA9550–17-1–039 and FA9550–17-1– 030, and NSF Grant No. PHY-2009999.
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Quantum geometric plasmonics: Berry curvature, quantum metric, and spontaneous collective mode ferromagnetism

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Plasmons, the self-sustained collective density modes in metals, form an integral part of the description of interacting electronic systems. Conventionally, plasmon dynamics are often dominated by the density and effective mass of carriers in its host metal. We will discuss how this description falls short in topological materials where the intricate twisting of wavefunctions (i.e. Bloch band quantum geometry) lead to a new class of plasmonic collective modes. These "quantum geometric" plasmons possess a wealth of exotic properties such as chirality even in the absence of magnetic field (in anomalous Hall metals) as well as bulk non- reciprocity of a quantum nature that persists even when classical non-reciprocity is absent (e.g., quantum metric plasmons).

Strikingly, when these wavefunction sensitive plasmons are driven out-of-equilibrium they can even exhibit dynamical symmetry breaking. As an example, we argue that when a non-magnetic metal (such as graphene) is driven by a linearly polarized (achiral) driving field, strong ac fields can enable the plasmons to spontaneously magnetize (acquire chirality). This out-of-equilibrium ferromagnetic phase is supported by "Berryogenesis": the spontaneous generation of a self-induced Bloch band Berry flux that supports and is sustained by a circulating plasmonic motion. These new plasmonic behaviors dramatically expand the phenomenology of interacting (quantum geometric) metals.

Funding: J.C.W.S. acknowledges support from the Ministry of Education, Singapore under its MOE AcRF Tier 3 Award No. 410 MOE2018-T3-1-002 and a Nanyang Technological University start-up grant (NTU-SUG).

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Multiconfigurational Approach to XAS applied to Ni- and Co-doped magnetide

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L-edge X-ray absorption spectroscopy (XAS) is an important tool to extract element- specific information about the electronic structure, magnetism and in particular electronic correlation effects. Ab initio calculations typically struggle to reproduce the 2p to 3d excitation, in particular for materials with strong electron correlations and significant core-hole effects. The combination of density functional theory and multiplet ligand field theory is applied to fill this gap. Here, parameters are calculated from first principles and used to construct a single-impurity Anderson model by projecting the local Hamiltonian and hybridization function onto the 3d states. In this talk, this method is applied to NiFe2O4, CoFe2O4 and Fe3O4. We find systematically good agreement with experiment for both XAS and XMCD spectra.

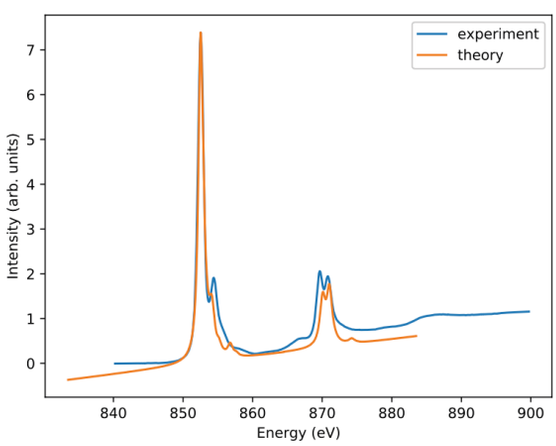

Figure 1: XAS of Ni in $NiFe_2O_4$

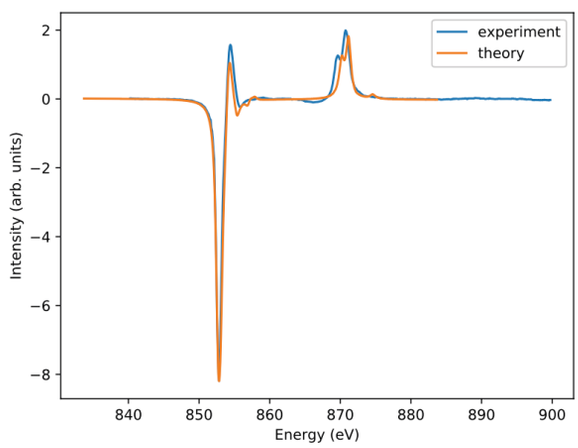

Figure 2: XMCD of Ni in $NiFe_2O_4$

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Spectral line shapes in dense plasmas

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Plasma coupling is defined as a ratio of the typical Coulomb to thermal energy in an ensemble of charged particles. This quantity can also be expressed through a ratio of two lengths, the mean inter-particle distance r0 and the Debye length λD. It is a crucial parameter governing various plasma properties. In particular, it enters expressions describing the ionization potential depression, which is important for modeling radiative properties of dense plasmas. There is, however, another quantity of the length dimension which is fundamental for describing discrete plasma spectra – the size of the atomic radiator a (i.e., a typical extent of the electron wave function). The "standard" multipole approach to the plasma line-shape modeling assumes the a/r0 and a/λD ratios to be negligibly small. In dense plasmas, however, this is no longer the case, resulting in important phenomena.

Here, we report on the first implementation of line-shape computer simulations accounting for the full Coulomb interaction directly. One benefit is the removal of inherent strong collision divergences in the multipole expansion approximation. Furthermore, it yields the plasma polarization shift produced by perturbers penetrating the wave function of the radiator bound electrons. The model was applied to hydrogenic argon Ly-α, Ly-β, and Ly-γ spectral lines in a dense argon plasma at free electron densities of 1024 or 1025 1/cm3 and temperature of 800 eV, relevant to plasma diagnostic techniques for inertial confinement fusion implosions.

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Speeding up X-ray-matter molecular dynamics simulation tool XMDYN with tree algorithms

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In molecular dynamics simulation method interactions between particles are numerically evaluated at each time-step. The interactions are either short-scale (involving only neighboring atoms, such as in case of chemical bonds) or long-range ones (i.e. in case of Coulomb interaction). While in the first case the computational cost scales with the number of particles N, the latter exhibits a scaling with N2. Therefore the evaluation of long-range interactions sets feasibility limits on system size. For the case of the Coulomb pair interactions several approximate methods (Barnes-Hut, Fast multi-pole, Ewald summation, etc.) were constructed for speeding up the calculations. In this work we are reporting on incorporating tree-code based schemes into the molecular dynamics code XMDYN [1]. The code XMDYN has been developed to describe interactions of X-rays with matter. We incorporated the tree- based Coulomb solver PEPC (Pretty Efficient Parallel Coulomb solver) [2] into XMDYN, and developed a dedicated tree based secondary ionization solver. These changes enable efficient simulations of X-ray irradiated large atomic assemblies, e.g. large protein systems or even viruses, that are of high interest for ultrafast X-ray science.

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Development of a new Quantum Trajectory Molecular Dynamics Framework

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The most common technique for modelling Warm Dense Matter (WDM) systems, DFT-MD, fundamentally does not consider electron dynamics. Therefore, there is a need for computational tools which explicitly evolve the electrons in time to investigate electron correlations and ion transport, predicted to be strongly influenced by electron dynamics [1]. We present an extension to the wave packet molecular dynamics scheme, applicable to WDM conditions [2], where the restricted functional form of the electron wave-packet allow for their non-adiabatic treatment over ion time scales. The extension introduces elongation in the wave packets for a better description of local non-isotropy and gradients in both disordered and molecular systems. Methods have been developed for the evaluation of Coulomb interactions, in terms of a generalised Ewald summation, and a pair-wise approximation of exchange effects, fully self- consistently with the extended functional form. The traditional treatment of Pauli interactions has been extended to include contributions due to interactions along the lines of Ref. [3]. The model has been implemented in the highly parallelised molecular dynamics framework LAMMPS to efficiently take advantage of existing computational resources and allow for the treatment of many-particle systems. The predictions from the newly developed code have been tested against other computational techniques for ground state energy of low-Z atoms and molecular hydrogen, electron-ion scattering compared with SOFT [4] and thermal electron density profiles tested against DFT predictions.

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Production of diamonds at the Facility for Antiprotons and Ion Research using intense heavy ion beams

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An important recent experiment using laser-compression of hydrocarbons has demonstrated phase separation of the material into hydrogen and, formation of diamond particles with a few nm diameter [1]. In this contribution we present numerical simulations that show that employing the intense uranium beam that will be available at the Facility for Antiprotons and Ion Research (FAIR) in the next couple of years, one can produce cylindrical diamonds with a length of a few mm and a diameter of around 400 – 500 micron. The beam-target geometry of the proposed experiment is presented in Fig. 1.

The target is comprised of a thin carbon cylinder that is enclosed in a tungsten shell. One face of the target is irradiated with an intense uranium beam having a circular focal spot and the beam axis coincides with the cylinder axis.

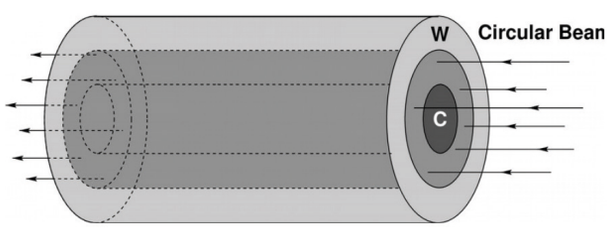

Figure 1: Beam-target geometry of the proposed experiment.

An appropriate ion energy (typically 1GeV/u) , is considered so that the ion range is larger than the cylinder length, and the Bragg peak lies outside the target. This leads to a fairly uniform energy deposition along the particle trajectory. Although the carbon sample is directly heated by the ion beam, the pressure in the surrounding heated part of the tungsten shell is higher than that in the carbon and hence the carbon is compressed. We have carried out extensive 2D hydrodynamic simulations using a wide range of the beam and the target parameters, which show that using appropriate beam intensity and focal spot size, it is possible to produce the necessary physical conditions to transform carbon into diamond. This experiment is an important part of the High Energy Density Physics program at FAIR that is named HEDP@FAIR [2].

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Large-scale structure prediction of near-stoichiometric magnesium oxide based on a machine-learned interatomic potential

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Using a fast and accurate neural network potential, we are able to systematically explore the energy landscape of large unit cells of bulk magnesium oxide with the minima hopping method [1]. The potential is trained with a focus on the near- stoichiometric compositions, in particular on suboxides, i.e., Mg_xO_{1-x} with $0.50 < x < 0.60$. Our extensive exploration demonstrates that for bulk stoichiometric compounds, there are several new low-energy rock-salt-like structures in which Mg atoms are octahedrally six-coordinated and form trigonal prismatic motifs with different stacking sequences.
Furthermore, we find a dense spectrum of novel nonstoichiometric crystal phases of Mg_xO_{1-x} for each composition of x. These structures are mostly similar to the rock-salt structure with octahedral coordination and five-coordinated Mg atoms. Due to the removal of one oxygen atom, the energy landscape becomes more glass-like with oxygen-vacancy type structures that all lie very close to each other energetically. For the same number of magnesium and oxygen atoms, our oxygen-deficient structures are lower in energy if the vacancies are aligned along lines or planes than rock-salt structures with randomly distributed oxygen vacancies. We also found the putative global minima configurations for each composition of the nonstoichiometric suboxide structures. These structures are predominantly composed of MgO(111) layers of the rock-salt structure which are terminated with Mg atoms at the top and bottom and are stacked in different sequences along the z direction. Like for other materials, these Magnéli-type phases have properties that differ considerably from their stoichiometric counterparts such as high electrical conductivity [2].

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Like-charge attraction in one- and two- dimensional Coulomb systems

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Like-charge attraction is the intriguing phenomenon when two particles with charges of the same sign that are immersed in an electrolyte turn out to have an effective interaction that is attractive instead of the natural expected repulsion. The effective interaction accounts for all the collective effects of the particles and the surrounding ions of the electrolyte. In this talk we will show how this phenomenon is indeed predicted in some one- and two-dimensional models of Coulomb systems [1, 2, 3, 4]. Exact analytical results can be obtained for these Coulomb systems models due to some connections that they have with integrable field theories. We will explain the techniques that allow to obtain exact results for the correlation functions between like- charge particles and how, under certain circumstances, the natural repulsion interaction shifts to being attractive. Although the technical details differ for 1d or 2d systems, the physical cause of this phenomenon is rooted in a three-body interaction between the like-charges and an ion of the electrolyte with opposite charge (Fig 1). This work was supported by Fondo de Investigaciones, Facultad de Ciencias, Universidad de los Andes INV-2021-128-2267.

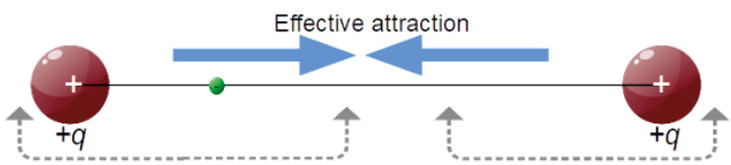

Figure 1: One ion (-) causes a charge imbalance between the (+) charges resulting in an attracting effective interaction.

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Classical Coulomb bridge functions in classical and quantum plasma liquids

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Central to the understanding of strongly coupled Coulomb systems are three idealized models: the classical one-component plasma (cOCP), quantum one-component plasma (qOCP) and Yukawa one-component plasma (YOCP). The models assume a strongly correlated charged species that is embedded in a rigid (cOCP, qOCP) or polarizable (YOCP) uniform charge neutralizing background. Their liquid state, although squeezed in a rather small portion of the phase diagram between the gas and the crystal states, has proven to be the most theoretically elusive due to its lack of small parameters.

The classical integral equation theory of liquids constitutes the most appropriate framework for the accurate computation of thermodynamic and static properties given its ability to retain information at all orders of the relative interaction strength. However, it requires an ad-hoc closure approximation for the bridge function, an enigmatic object of diagrammatic analysis whose virial type expansion is impossible to calculate, and whose extraction from simulations is quite formidable and relatively unexplored.
We present a general methodology for the indirect extraction of bridge functions $BB(rr)$ from molecular dynamics (MD) simulations. The intermediate and long range $BB(rr)$ is obtained by employing the Ornstein-Zernike inversion method with input from standard NVT MD simulations, while the short range $BB(rr)$ is obtained by employing the cavity distribution method with input from specially designed NVT MD simulations featuring a tagged particle pair [1]. This methodology is applied to the cOCP, after system – specific peculiarities such as the Ewald sum and compressibility sum rule are considered [2]. The bridge function is extracted for 17 cOCP states spanning the dense liquid region and is accurately parametrized with a switching function strategy [2,3]. This input leads to a near-exact solution of the structural and thermodynamic problem for the cOCP.

In addition, the cOCP bridge function is used as input in the novel isomorph-based empirically modified hypernetted chain (IEMHNC) approach for the YOCP [4]. The cOCP bridge functions are "one-to-one" mapped to YOCP bridge functions along isentropic phase diagram lines, based on the bridge function isomorph invariance property of R- simple systems such as the YOCP [1]. The IEMHNC approach leads to structural and thermodynamic predictions that have a truly unprecedented accuracy on par with that of computer simulations [2]. Finally, the cOCP bridge function is used as an input in a novel integral equation theory based dielectric scheme for the qOCP [5]. Comparison with ab initio path integral Monte Carlo simulations of the paramagnetic electron liquid revealed an excellent agreement especially in terms of the interaction energy and the long wavelength limit of the static local field correction [5].

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Phase separation/diagram of dusty plasmas

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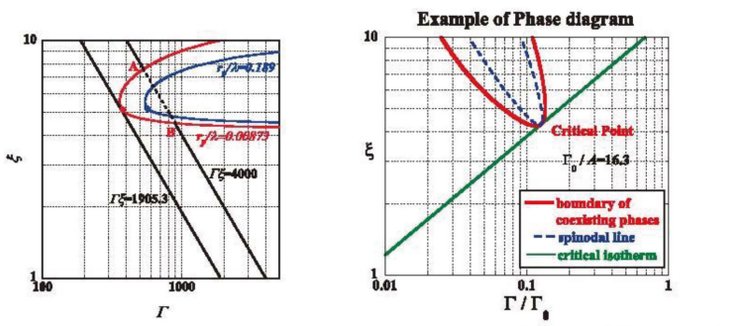
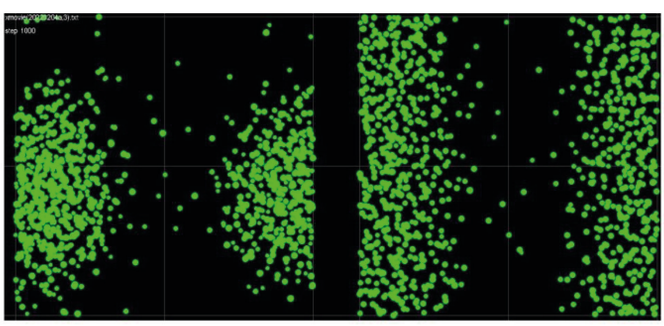
Fine particles (dusts) of micron sizes in weakly ionized plasmas have large negative charges and form a strongly-coupled Yukawa system. Coupling parameter Γ can reach 10^3 with screening length λ around mean distance a ($\xi=a/\lambda$) . The whole system including electrons and ions has been predicted to be thermodynamically unstable when strongly coupled, leading to phase separations [1,2]: Two phases co-exist Inside of curves at strong (left) and extremely strong (right) coupling.



Note the change in Γ-dependence of isotherms; $\xi \propto \Gamma^{-1} \rightarrow \xi \propto \Gamma^{1/2}$ $(A \sim 10^5)$.

Numerical simulations have been performed for systems composed of Yukawa particles and electron-ion plasma, the latter being treated as continuum. Shown below is an example.



These phenomena are also expected for Yukawa mixtures and may be observed in experiments on the ground with appropriate considerations on the effect of gravity.

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First principles thermodynamic simulations of dense two-component plasmas: combining configuration PIMC and permutation blocking PIMC approaches

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Path integral Monte Carlo (PIMC) simulations of dense plasmas are severely hampered by the notorius fermion sign problem. We have recently achieved first- principle results for the warm dense electron gas that avoid the fixed node appro- ximation by combining two complementary methods: configuration PIMC [1] and permutation-blocking PIMC [2] which were first published in Ref. [3]. In this contribution we discuss how this combination of methods can be extended to two-component plasmas. We expect that this will allow for an extension of direct fermionic PIMC si- mulations [4, 5] to strong degeneracy.
Acknowledgements: This work is supported by the DFG via project BO1366/15.

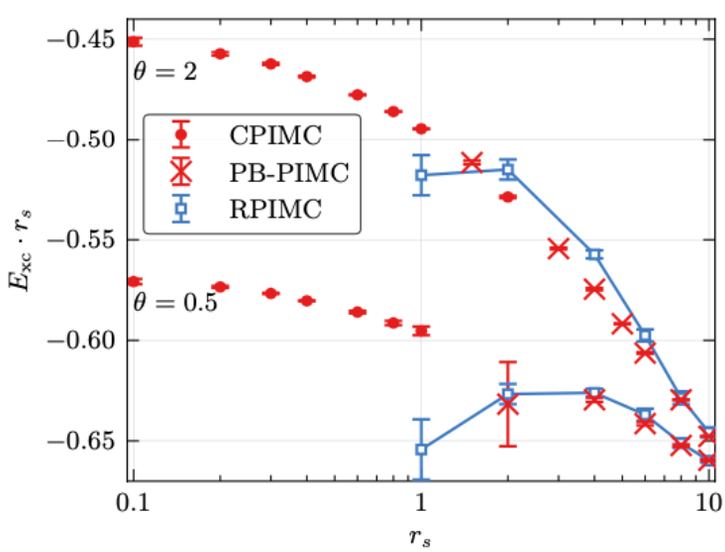

Figure 1: Exchange-correlation energy for 33 spin polarized electrons at half the Fermi tempera- ture. First principle CPIMC and PB-PIMC results smoothly merge whereas fixed node QMC results (blue) fail. From Ref. [3].

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Eliashberg theory of superconductivity from electronic collective excitations

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The Eliashberg equation for the anomalous self-energy of the superconducting state is a powerful tool for the study of superconductivity by both conventional (electron- phonon) and unconventional (purely electronic) mechanisms. In the latter case, however, Migdal's theorem on the unimportance of vertex correction fails and care must be exerted in constructing the effective electron-electron interaction. In this talk I review theoretical studies of purely electronic superconductivity which I have been involved with over the years in systems as diverse as the electron hole liquid1, the two- dimensional electron gas2, and twisted bilayer graphene3. Vertex corrections (included approximately in the form of local field factors) drive superconductivity in the first case, suppress it in the second, and have not yet been evaluated in the third.

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FermiFlow: a variational free-energy approach for fermions in the continuum

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Nature tries to bring physical systems into a minimal free energy state via balancing their energy and entropy. Ironically, it is difficult to turn such a free energy minimization principle directly into a practical simulation algorithm, especially for fermions in the continuum. One of the difficulties is the prohibitive cost associated with the entropy contribution in the free energy, known as the "intractable" partition function problem. The latest advances in deep learning have brought us a large family of neural network-based generative models that are tractable yet flexible enough to represent, learn, and sample from high-dimensional probability distributions.
In FermiFlow, we represent the variational density matrix of fermions in the continuum using two deep generative models: an autoregressive model for the normalized classical Boltzmann distribution and a permutation equivariant normalizing flow for the orthonormal quantum states. Joint optimization of the two models under the free-energy principle solves interacting fermions at finite- temperature variationally. As a first application, we employ the approach to investigate low-temperature entropy of uniform electron gases, which provides a direct estimate of quasiparticle effective mass for the Fermi liquid theory.

Hao Xie, Linfeng Zhang, Lei Wang, arXiv: 2105.08644 and 2201.03156, https://github.com/fermiflow/

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Coulomb gas sum rules for vortex-pair fluctuations in 2D superfluids

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Coulomb-gas sum rules are used to characterize thermal vortex-pair fluctuations in 2D superfluids. Simulations of the 2D XY model have been carried out to study the net winding number of vortices at a given temperature in a circle of radius R. At all temperatures the average net squared winding number <W2> is found to scale as a perimeter law, linear in R, in agreement with Coulomb-gas theories [1], and at infinite temperature agrees nearly exactly with an early theory by D. Dhar [2] . Figure 1 shows the slope of the perimeter law as a function of temperature, showing a sharp peak near 1.15 TKT, very similar to the peak in specific heat. The red triangles in the figure are the prediction of a Coulomb-gas sum rule [1] for the slope, computed from an integral of the vortex- vortex distribution functions below the Kosterlitz-Thouless superfluid onset temperature TKT. The sum rule cannot be computed above that temperature since the vortex distribution functions are no longer the same as the vortex- vortex correlation functions. The red cross at infinite temperature is the Dhar theory prediction [2] of a slope of 2.0, precisely the value we find.

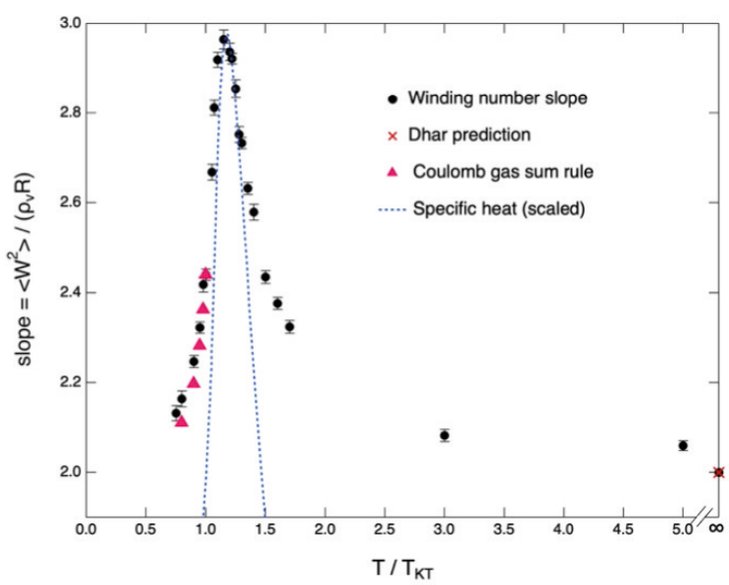

Figure 1: Slope of the perimeter law fluctuations of vortex pairs in the 2D XY model.

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Towards Large-Scale and Spatio-temporally Resolved Diagnosis of Electronic Density of States by Deep Learning

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Modern laboratory techniques like ultrafast laser excitation and shock compression can bring matter into highly nonequilibrium states with complex structural transformation, metallization and dissociation dynamics [1-4]. To understand and model the dramatic change of both electronic structures and ion dynamics during such dynamic processes, the traditional method faces difficulties.
Here, we demonstrate the ability of deep neural network (DNN) to capture the atomic local-environment dependence of electronic density of states (DOS) for both multicomponent system under exoplanet thermodynamic condition and nonequilibrium system during super-heated melting process [5]. Large scale and time-resolved diagnosis of DOS can be efficiently achieved within the accuracy of ab initio method. Moreover, the atomic contribution to DOS given by DNN model accurately reveals the information of local neighborhood for selected atom, thus can serve as robust order parameters to identify different phases and intermediate local structures, strongly highlights the efficacy of this DNN model in studying dynamic processes.

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Screw dislocation defect filaments in quenched Yukawa liquids under confinements

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The screw dislocation defect with a helical front winding around a line is an important structural singularity commonly occurring in various systems, such as 3D crystals [1], nacreous structures [2], and wave media [3]. For cold liquids under flat confinement, layered structures can be formed through the suppression of the transverse motion by the boundary. Previous studies on liquids under confinement have investigated the crystallization [4], 3D structure [5], and intralayer structural evolution [6]. In this work, using the confined and quenched 3D Yukawa liquid as a platform, we numerically demonstrate the first observation of the screw dislocation defects with wiggling filament-like cores and investigate their dynamics.

It is found that, pairs of worm-like defects winded around by screw-type layers with opposite helicities can be spontaneously generated. It forms a chaotic defect filament network in the 3D space. The increasing layering order with increasing time after quenching decreases filament number density through defect pair annihilation. The spatiotemporal evolutions of defect filaments and the surrounding stereo layering fronts are presented and discussed.

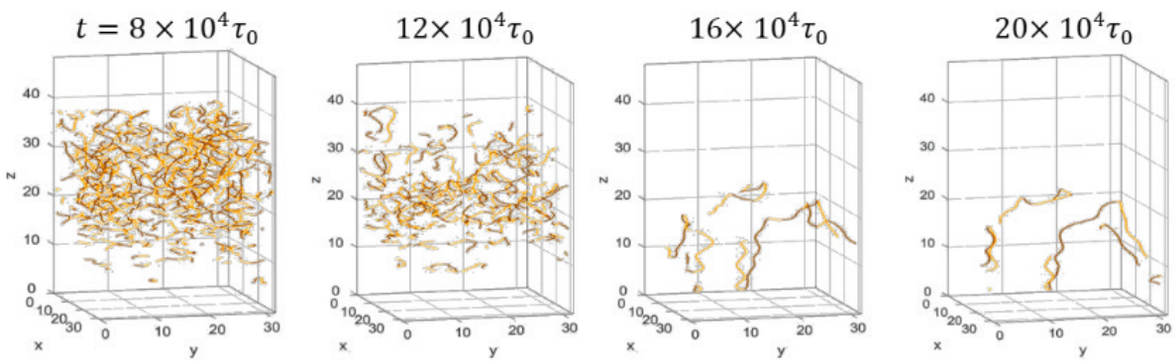

Figure 1: Spatiotemporal evolution of defect filaments. Yellow (brown) colors represent right (left) handed screw dislocation defect filaments. With increasing time, the number of defect filament decreases, and the defect loops are formed.

[1] P. M. Chaikin, T. C. Lubensky, and T. A. Witten, Principles of condensed matter physics. Cambridge: Cambridge university press. (1995).
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Percolation transition of layering in 3D Yukawa liquids under confinement

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For the liquid under confinement, the topological constraint of the flat boundary lines up the particle and leads to the formation of adjacent layered structure, which can be deteriorated by the background thermal agitation. As the distance normal to the boundary decreases, the disordered micro-structure transits to the ordered layered structure. Whether this transition belongs to the general category of the phase transition governed by percolation theory in various nonlinear extended systems, such as turbulent puffs in hydrodynamic turbulence [1], forest fire [2], and epidemic spread [3], is still unexplored. Here, we numerically investigate the above unexplored issue in a confined 3D Yukawa liquid. It is found that, the fraction of area occupied by layered sites exhibits a smooth rapid transition with decreasing distance normal to the boundary. Layered sites emerge in the form of multi-scale clusters exhibiting power- law cluster size distributions, with gradually increasing scaling exponents before forming a large percolating cluster spanning over the system. Similar percolating transition behaviors can also be observed of the sites using good intra-layer structural order as a local order parameter, and the layering transition behaviors by decreasing temperature for a layer with a fixed distance from the boundary. Our observed transition behaviors are all similar to those of the transitions in non-equilibrium systems governed by percolation theory.

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Anomalous Josephson effect in chiral double layers

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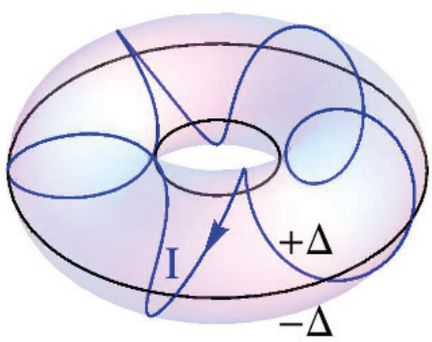
We consider s-wave pairing in a double layer of two chiral metals due to inter- layer Coulomb interaction,and study the Josephson effect near a domain wall, where the sign of the order parameter jumps. The domain wall creates two evanescent modes at the exceptional zero-energy point, whose superposition is associated with currents flowing in different directions in the two layers. Assuming a toroidal geometry, the effective Josephson current winds around the domain walls, whose direction is determined by the phase difference of the complex coefficients of the superimposed zero-energy modes. Thus, the zero-energy mode is directly linked to a macroscopic current. This result can be understood as an interplay of the conventional Josephson current perpen- dicular and the edge current parallel to a domain wall in a double layer of two chiral metals. As a realization we suggest the surface of a ring-shaped topolo- gical insulator. A duality between electron-electron and electron-hole double layers indicates that this effect should also be observable in excitonic double layers.



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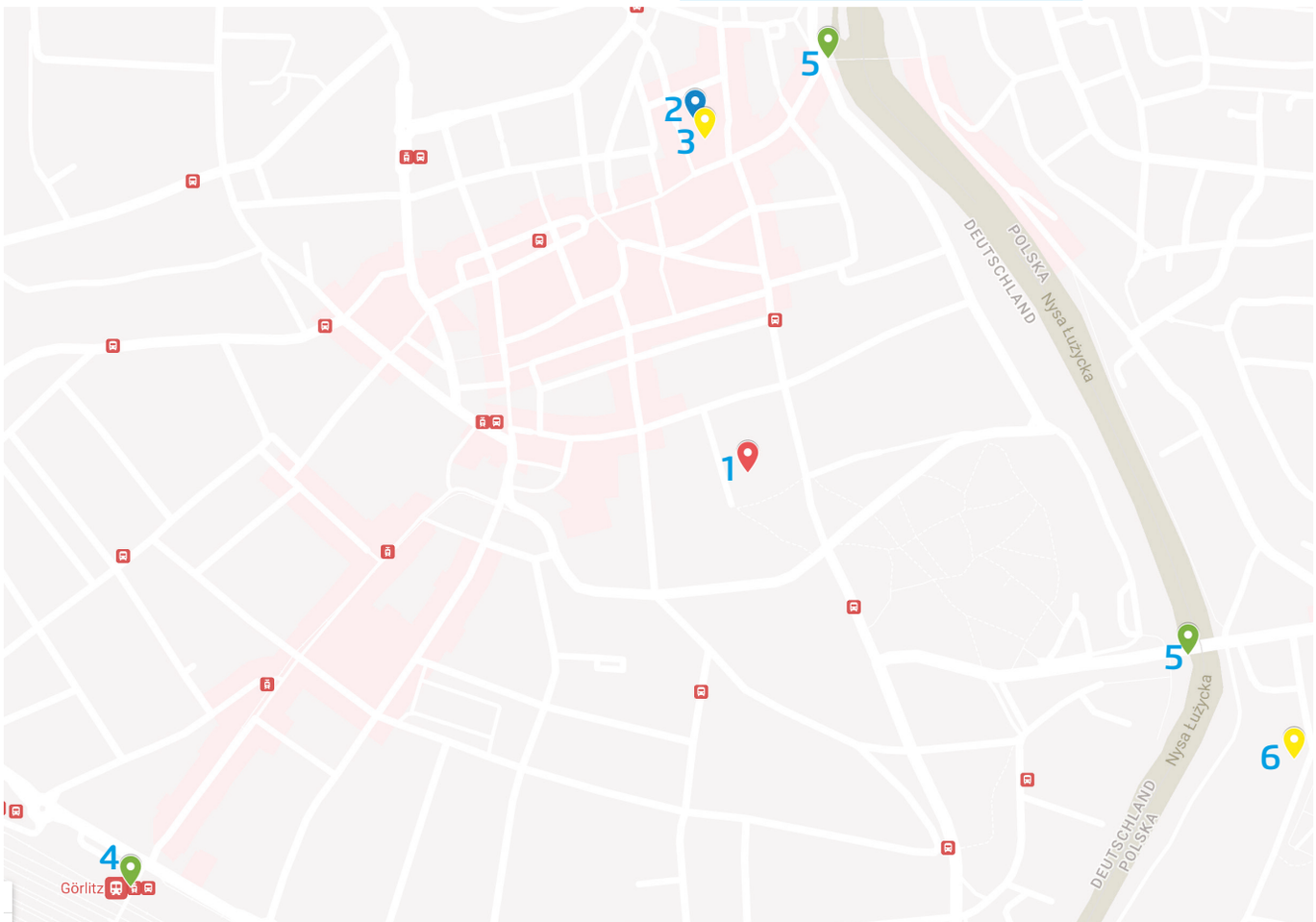
GOOD TO KNOW

AREA MAP



1 Synagogue Görlitz - conference venue (Otto-Müller-Straße 3)
2 Center for Advanced Systems Understanding CASUS (Untermarkt 20)
3 Hotel Börse (Untermarkt 16)
4 Train Station Görlitz (Bahnhofstraße 76)
5 Bridge Germany-Poland
6 Restaurant “Villa Toro” - conference dinner (Wolności 9, Zgorzelec)

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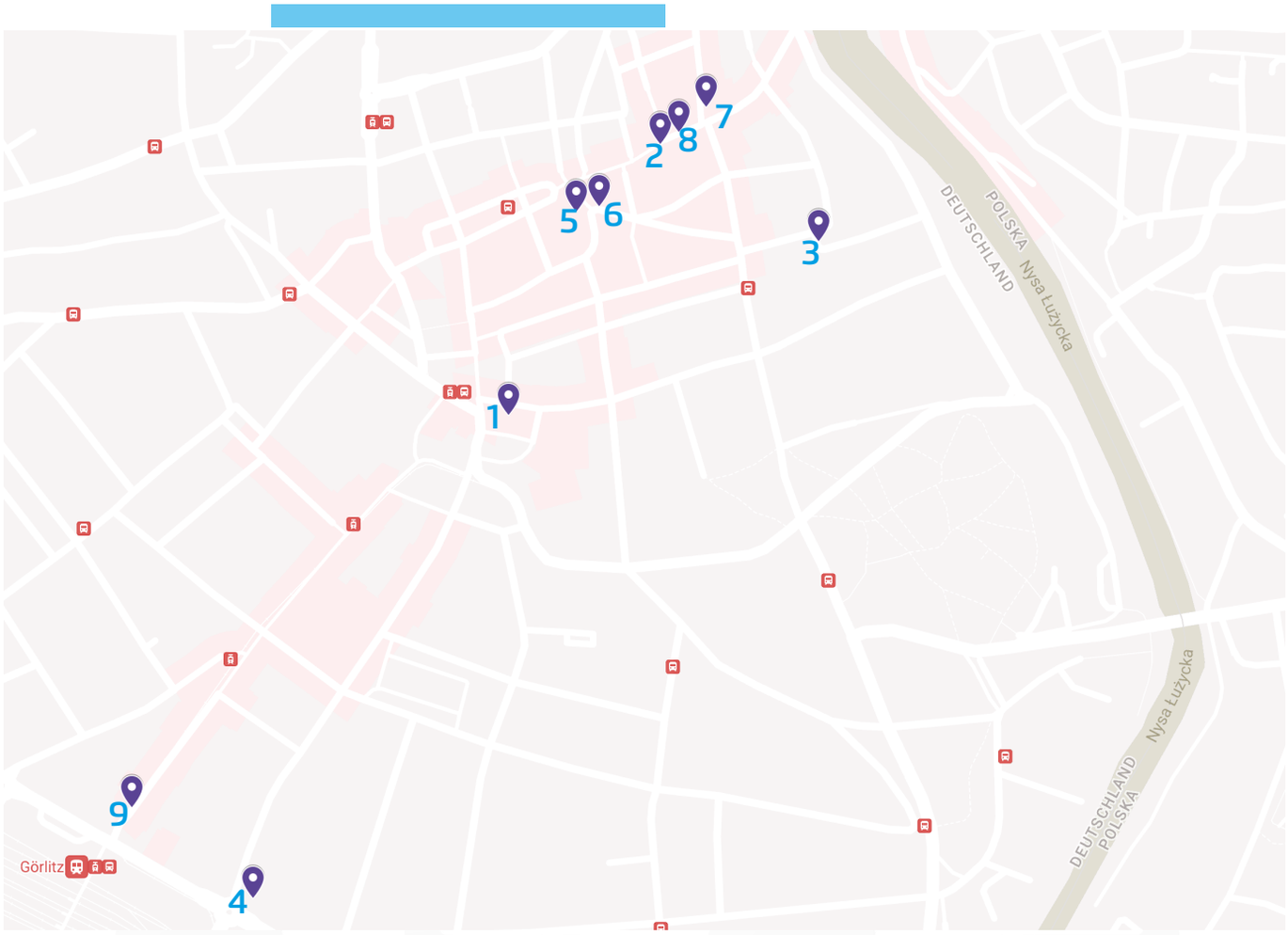
GOERLIWOOD MAP



1 Kaufhaus Görlitz
2 Brüderstraße
3 Bergstraße
4 Filmpalast Görlitz
5 Dreifaltigkeitskirche
6 Fischmarkt
7 Untermarkt 25
8 Untermarkt 5
9 Berliner Straße

Original places in Görlitz

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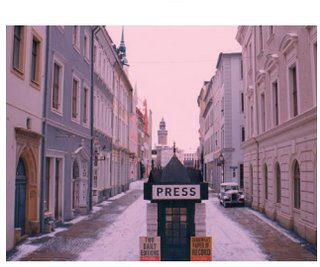
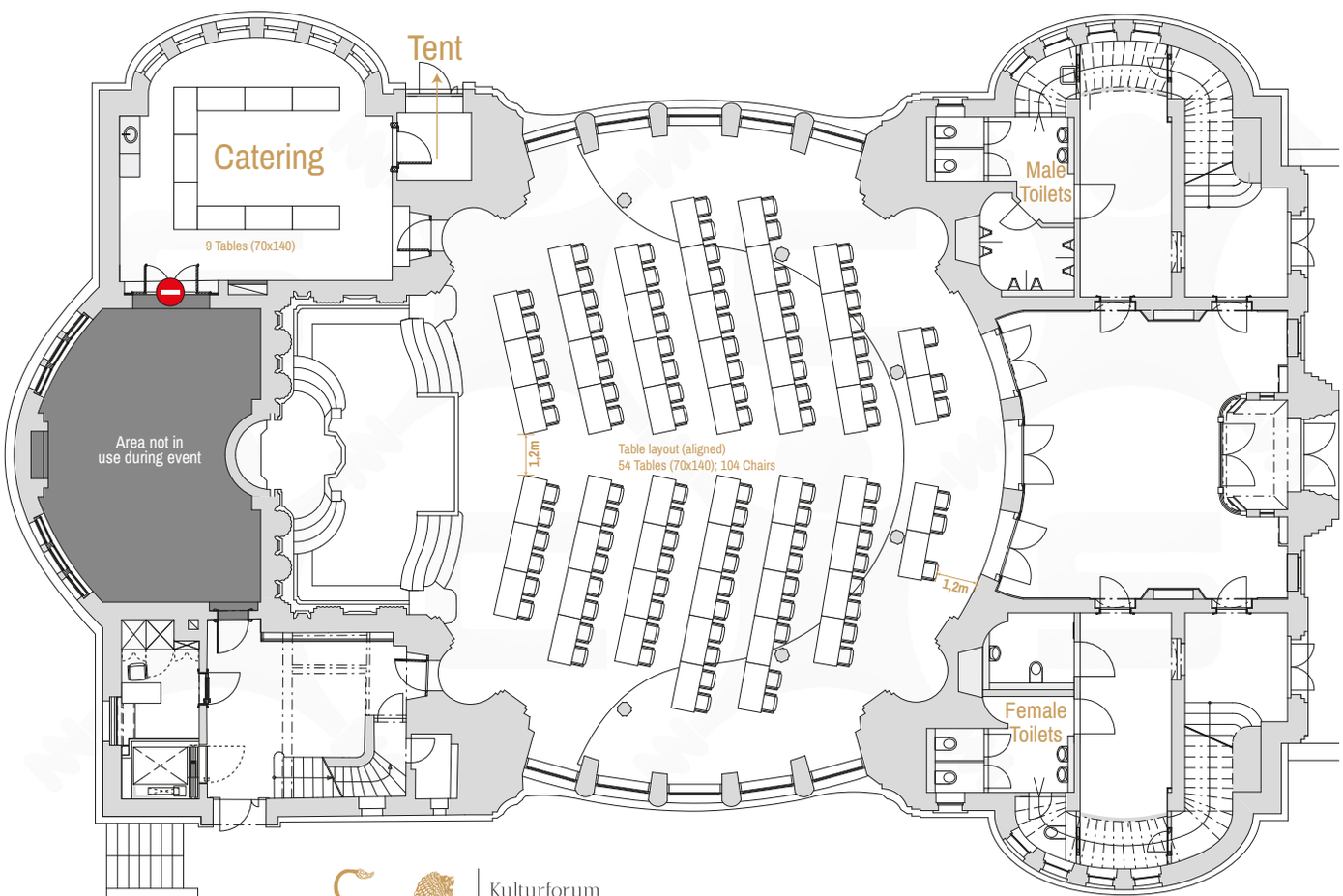


Locations in “Grand Budapest Hotel” movie

PLAN OF SYNAGOGUE



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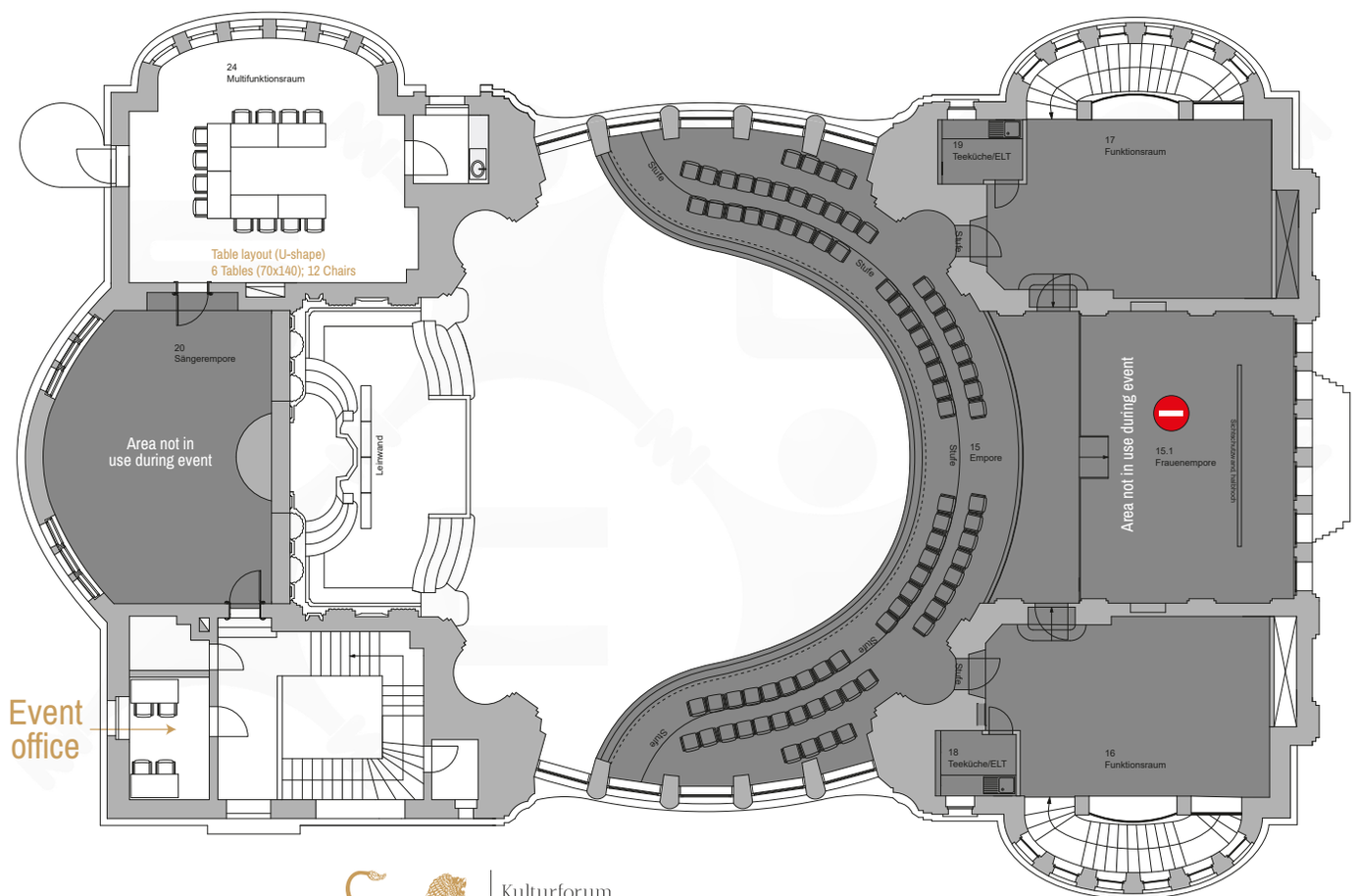

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Kulturforum Görlitzer Synagoge - Konferenzbestuhlung

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Floorplan upper level - Empore

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