International Conference

Strongly Coupled Coulomb Systems

30 July – 4 August 2017, Kiel

Keynote Speakers

Gordon Baym (Illinois, USA)
Siegfried H. Glenzer (Stanford, USA)
Stefan Kuhr (Strathclyde, UK)
Stephane Mazevet (Paris, France)
Carlo Pierleoni (L'Acquila, Italy)
Andrea Tomadin (Genoa, Italy)

Invited Speakers

Bernard Bernu (Paris, France)
Ben van Duppen (Antwerp, Belgium)
Tobias Dornheim (Kiel, Germany)
Yan Feng (Soochow, China)
V.E. Fortov (Moscow, Russia)
Martin French (Rostock, Germany)
Fabian Heirich-Meisner (Munich, Germany)
Y.E. Lozovik (Moscow, Russia)
Manoel Manghi (Toulouse, France)
Andrea Perali (Camerino, Italy)
Alessandro Principi (Nijmegen, Netherlands)
Niclas Schlünzen (Kiel, Germany)
Luciano Silvestri (Boston, USA)
Jan Vorberger (Dresden, Germany)
Ulf Zastrau (Hamburg, Germany)

Local Organizing Committee SCCS 2017
Michael Bonitz, Patrick Ludwig & Zhandos Moldabekov
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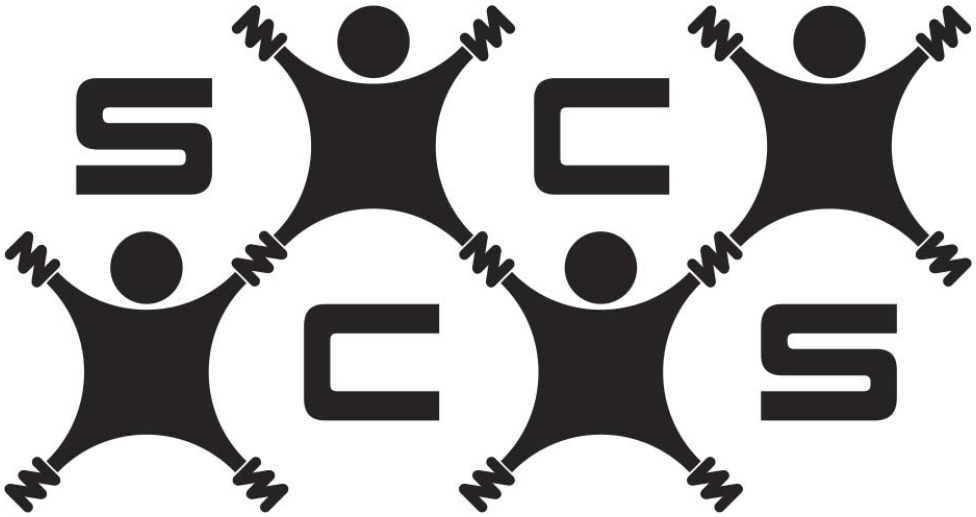


STRONGLY COUPLED COULOMB SYSTEMS

Final Program & Book of Abstracts

Kiel, July 30–August 4, 2017
Wissenschaftszentrum Kiel

Topics of SCCS 2017

1. Dense and astrophysical plasmas
2. Plasmas in condensed matter
3. Confined and mesoscopic Coulomb systems
4. High-energy-density plasmas in the laboratory
5. Classical charged systems
6. Developments in theoretical methods and numerical techniques
7. Dynamics of correlated quantum Coulomb systems

Conference website
http://www.uni-kiel.de/sccs2017

Welcome to SCCS 2017

'Strongly Coupled Coulomb Systems' (SCCS) is a major series of international conferences for scientists drawn from a large variety of fields including plasma physics, astrophysics and condensed matter physics. In all these fields the behavior of charged many-particle systems and the role of their correlations play a central role, and many results from one area have been found useful in other areas as well. The idea of a conference bringing together experts from such diverse fields is due to Gabor Kalman who organized the first meeting in 1977. 40 years back it was not foreseeable that this would become such a successful conference series.

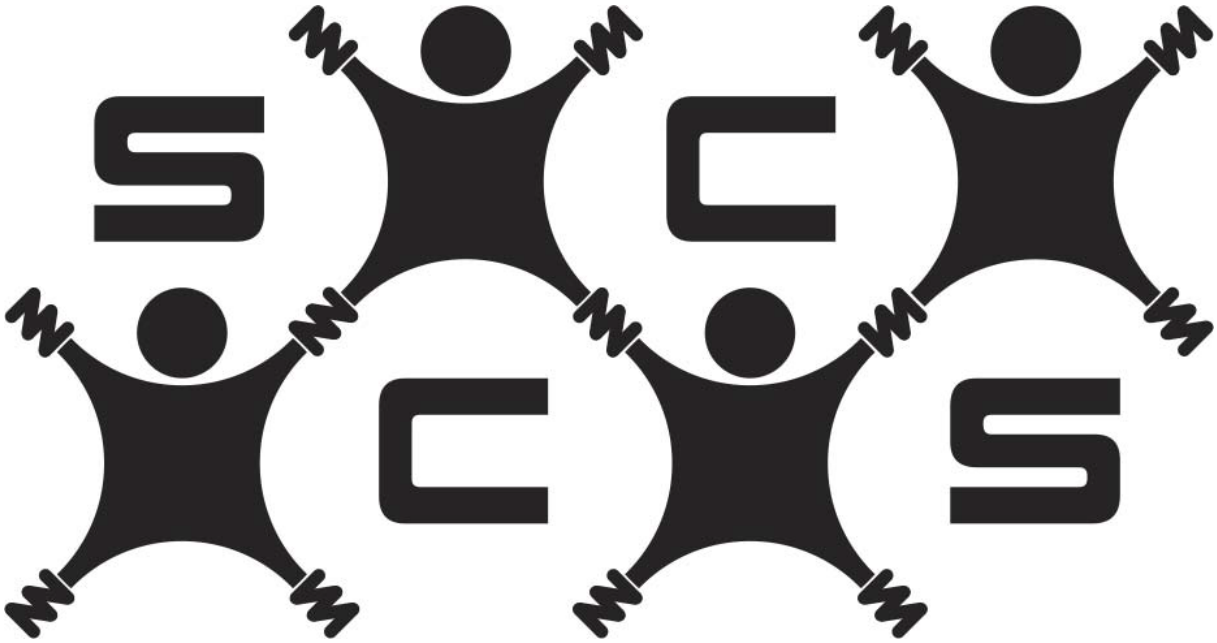
In the mean time the SCCS conferences have become an important event held in 3 years intervals in locations all over the world. The goal is to provide a regular international forum for the presentation and discussion of research achievements and ideas relating to a variety of plasma, liquid and condensed matter systems that are dominated by strong Coulomb interactions between their constituents. Each meeting has seen an evolution of topics that have followed in the steps of new discoveries and new methods. In recent years the field has seen the emergence of new experimental tools and access to new strongly coupled conditions including e.g. dusty plasma, ultracold neutral plasmas. Each time novel topics emerge. This time these are the topics of dynamics of correlated quantum systems, including cold fermionic atoms and plasma-surface interaction.

The program committee and the local organizers have managed to form an excellent and exciting collection of talks and posters, and we have created best possible conditions for a stimulating exchange of ideas. The conference has attracted a very diverse international group of researchers – from leading experts with long research experience – to the next generation: young scientists and students. To support participants financially, the organizers have obtained substantial funds from the German Science Foundation (DFG) and Kiel University (KiNSIS). But we are equally grateful to our keynote and invited speakers who have returned part of our travel support in order to make participation of young researchers possible.

We wish all participants a successful SCCS conference and a memorable stay in Kiel.

Michael Bonitz, Patrick Ludwig & Zhandos Moldabekov
Local organizing committee

SCCS 2017
Conference Schedule



Monday, July 31

08:30 Opening

Session I: Dense and astrophysical plasmas

10:15 Coffee break and informal discussions

Session II: Classical charged particle systems

12:30 Lunch and informal discussions

Session III: Dynamics of correlated quantum Coulomb systems

16:15 Coffee break and informal discussions

Poster introductions and poster session I

16:30–18:00

Tuesday, August 1

Session IV: Dense and astrophysical plasmas

10:15 Coffee break and informal discussions

Session V: Confined and mesoscopic Coulomb systems

12:30 Lunch and informal discussions, IAB meeting

Session IV: Dynamics of correlated quantum Coulomb systems

16:15 Coffee break and informal discussions

Poster introductions and poster session II

16:30–18:00

Historical remarks

17:45 W. Ebeling

What is the correct choice of the plasma partition function and the lowering of the ionization energy–on contributions by Planck and Unsöld 52

Wednesday, August 2

Session VII: High-energy-density plasmas in the laboratory

08:45 S.H. Glenzer
[keynote] *Ultrafast probing of dense plasmas–visualizing dynamics of Strongly Coupled Coulomb Systems* 53

09:30 D.H.H. Hoffmann
Accelerator driven high energy density science: status of HED physics at FAIR and GSI 54

09:45 T. Döppner
Ionization measurements in 30-fold compressed, near-degenerate plasmas . 55

10:00 G. Norman
Ionization of molecules at the fluid-fluid phase transition in warm dense hydrogen 56

10:15 Coffee break and informal discussions

Session VIII: Confined and mesoscopic Coulomb systems

10:45 A. Perali
[invited] *Strong electron correlations in graphene and related materials* 57

11:15 E.H. Hwang
Coupled plasmon modes in vertically stacked 2D nanomaterials 58

11:30 H. Totsuji
Strongly coupled fine particle clouds in fine particle plasmas 59

11:45 H. Pan
Strongly coupled dusty plasma in a 2D harmonic trap 60

12:00 P. Hartmann
Diffusion in two-dimensional quasi-magnetized rotating dusty plasmas 61

12:15 K. Müller-Dethlefs
Observation of a periodic many-body system 62

12:30 Lunch and informal discussions

Conference excursion to Lübeck

14:00–20:00

Thursday, August 3

Session IX: Developments in theoretical methods and numerical techniques

08:45 C. Pierleoni
[keynote] *Coupled electron-ion Monte-Carlo methods for warm dense hydrogen* 63
09:30 T. Dornheim
[invited] *Ab initio Quantum Monte Carlo results for the warm dense electron gas* . . . 64
10:00 F. Heidrich-Meisner
[invited] *Nonequilibrium dynamics in the Hubbard model* 65

10:30 Coffee break and informal discussions

Session X: High-energy-density plasmas in the laboratory

11:00 V.E. Fortov
[invited] *Quasi-adiabatic multi-shock compression of strongly coupled plasmas: correlations and degeneracy* 66
11:30 D.N. Nikolaev
Brightness temperature and specific conductivity of multiple shocked initially gaseous protium and deuterium up to 0.4 TPa 67
11:45 U. Zastrau
[invited] *High energy density plasmas diagnosed with X-ray free electron lasers* 68
12:15 P. Sperling
Exploring the physical properties of warm dense water by using Free-Electron-Laser 69

12:30 Lunch and informal discussions

Session XI: Electron liquids and complex plasmas

14:30 A. Principi
[invited] *Viscosity, thermal conductivity and violation of the Wiedemann-Franz law in hydrodynamic electron liquids* 70
15:00 A. Bataller
2D plasma condensation in monolayer semiconductors 71
15:15 L. Silvestri
[invited] *Collective behavior of Yukawa systems* 72
15:45 T.S. Ramazanov
Structural and dynamic properties of strongly coupled dusty plasma of RF discharges 73
16:00 H. Charan
Bow shock formation by supersonic flows in the presence of an obstacle in a two dimensional strongly coupled complex plasma 74

16:15 Coffee break and informal discussions

Poster introductions and poster session III

16:30–18:00

Conference dinner

19:30–23:00

Friday, August 4

Session XII: Plasmas in condensed matter

10:15 Coffee break and informal discussions

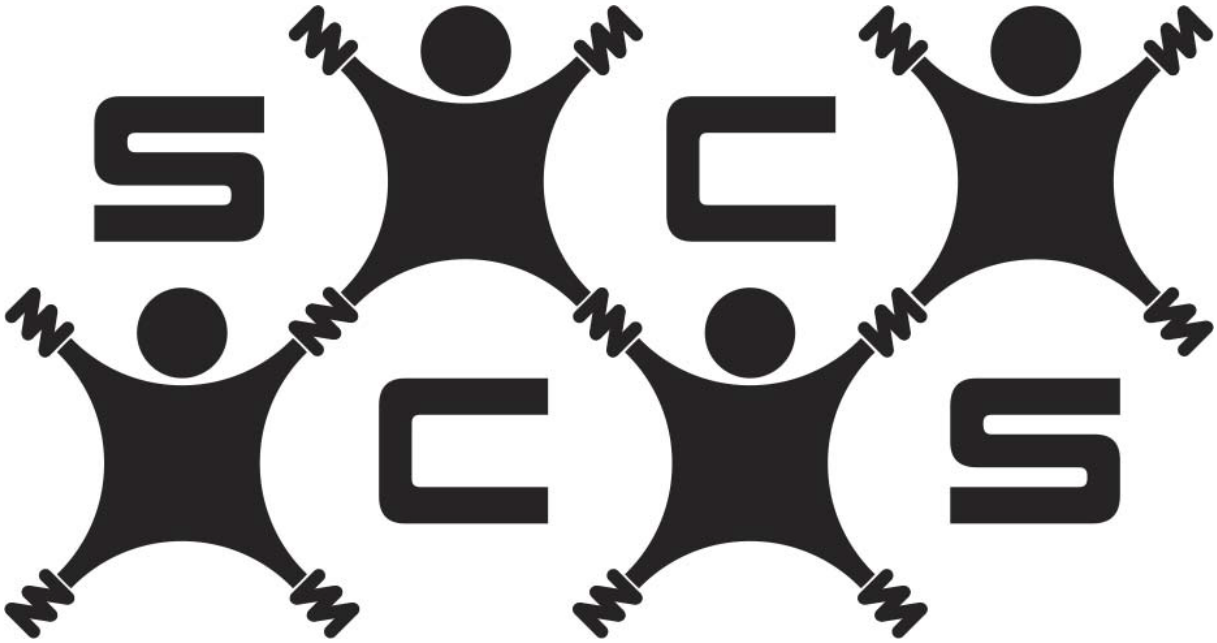
Session XIII: Transport properies of dense plasmas

12:30 Lunch and informal discussions

Session XIV: Thermodynamics of strongly coupled plasmas

15:00 Concluding discussion. Closing remarks

List of Posters



Monday

Poster Session I

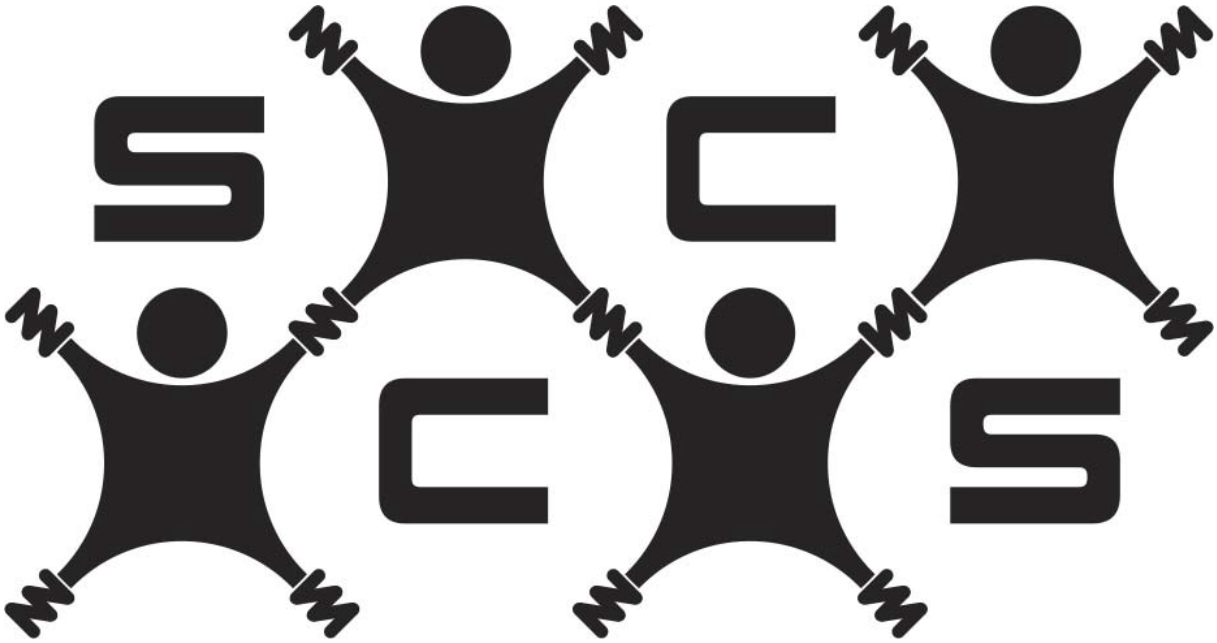
Tuesday

Poster Session II

Thursday

Poster Session III

Oral Presentations



Ab initio equation of states for planetary and exoplanetary modeling

S. Mazevet[*1,3], T. Tsuchiya[2], R. Musella[1], J. Bouchet[3], V. Recoules[3], F. Guyot[4], G. Morard[4], A. Benuzzi-Mounaix[5,1], A. Licari[6], F. Soubiran[6], G. Chabrier[6]

[1] LUTH, UMR8102, Observatoire de Paris, CNRS, PSL Resrach University, Université Paris Diderot, 5 place Jules Janssen, 92190 Meudon Cedex France
[2] Geodynamics Research Center, Ehime University, 2-5 Bunkyo-cho, Matsuyama, Ehime 790-8577, Japan, and Senior Research Fellow Center, Ehime University, 2-5 Bunkyo-cho, Matsuyama, Ehime 790-8577, Japan
[3] CEA, DAM, DIF, F-91297 Arpajon, France
[4] IMPMC, UPMC, UMR CNRS 75-90, Sorbonne Université Paris, France
[5] LULI, Ecole Polytechnique, CNRS, CEA, UPMC, route de Saclay, 91128 Palaiseau, France
[6] Ecole normale supérieure de Lyon, CRAL, UMR CNRS 5574, Université de Lyon, 69364 Lyon Cedex 07, France

Using ab initio molecular dynamics simulations, we recently calculated equations of state for the main constituents of planetary interiors: H, He, H_2O, $MgSiO_3$(MgO,SiO_2) and Fe. These equations of states are multi-phases, include liquid and solid phases, and aim at building planetary and exoplanetary interior models solely based on ab initio predictions. This talk will concentrate on Jupiter. We will review how our current understanding of the behavior of these basic constituents at extreme density temperature conditions has modified our current understanding of Jupiter interior, not only for the envelop where metallization of hydrogen and hydrogen-helium demixing is the issue but also for the core where the high pressure melting properties of iron, water and silicates bring a new understanding on the nature of giant planet cores.

This work is supported in part by the French Agence National de la Recherche under contract PLANETLAB ANR-12-BS04-0015 and the PSL IRIS project Origins and Conditions for the Emergence of Life.

[1] L. Caillabet, et al., Phys. Rev. B **83**, 094101 (2011).
[2] F. Soubiran et al., Phys. Rev. B **87**,165114 (2013).
[3] J. Bouchet et al., Phys. Rev. B **86**, 115102 (2013).
[4] A. Denoeud et al., Phys. Rev. Lett. **113**, 116404 (2014).
[5] S. Mazevet et al., Phys. Rev. B **92**, 014105 (2015).
[6] M. Harmand et al., Phys. Rev. B **92**, 024108 (2015).
[7] A. Denoeud et al., Phys. Rev. E, accepted (2016).

* email: stephane.mazevet@obspm.fr

Thermodynamics of deuterium at terapascal pressure range

V.K.Gryaznov[1,2], I.L.Iosilevskiy[3,4]

[1]Institute of Problems of Chemical Physics RAS, 142432, Chernogolovka, Russia
[2]National Research Tomsk State University, Tomsk, 634050, Russia
[3]Joint Institute for High Temperatures RAS, 125412, Moscow, Russia
[4]Moscow Institute of Physics and Technology (State University), 141700, Dolgoprudnyi, Russia

Equation of state of deuterium at submegabar and megabar ranges of pressures and high temperatures were experimentally studied with different methods. At these parameters where a high density of matter is accompanied by a strong Coulomb interaction (strongly non-ideal plasma) thermodynamic properties of gases have been theoretically described both as in frames of the chemical picture (free energy minimization model) so with the ab-initio methods involving the direct numerical simulation of system of nuclei and electrons. In spite of achievements of experimental and theoretical methods in this range of parameters further study of dynamically compressed light gases is important. In particular, the problem of the possibility of a phase transitions at high compression degrees is not resolved yet. The experimental data on caloric and thermal equation of state cover pressures of shock and isentropic compression from kilobars to dozen megabars and rather high densities. Last several years new theoretic results in frames of chemical picture and ab-initio methods in a wide range of pressures generated with shock and quasiisentropic compression have been presented as well.

Here we present the results of calculation of equation of state of quasiisentropically compressed deuterium up to pressures about 10 terapascal and density about 10 g/cc. These calculations were carried out with codes implemented the improved SAHA-family models.

The calculations have shown that in the considered pressure range dynamically compressed deuterium is in a state of strongly coupled, highly degenerated plasma. Results of our calculations are compared with those obtained in frames of the first principal quantum methods and of newest experimental data.

Miscibility gap of hydrogen-helium mixtures

Manuel Schöttler*, Ronald Redmer

Universität Rostock, Germany

We determine the demixing phase diagram of hydrogen-helium mixtures at high pressures, which is important for applications in planetary physics, in particular, for calculating the interior and evolution of gas giants. Hydrogen-helium demixing has long been proposed as a possible source of Saturn's excess luminosity: The initially hot planet cools down with increasing age and when the planetary isentrope enters the demixing region, helium-rich droplets can form and sink toward the planetary core, thus, acting as an additional source of heat; see, e.g., [1].
The region of demixing is observed from thermodynamic relations by computing the free enthalpy G(x,P,T) at constant pressure P and temperature T for different helium fractions x. We use finite-temperature density functional theory molecular dynamic simulations to obtain the equation of state for given volumes and temperatures including the non-ideal entropy of mixing.
The choice of an exchange-correlation (XC) functional, that captures the relevant physics, is of paramount importance. It has been shown that standard approximations such as PBE lack the ability to adequately describe the metallization transition in hydrogen [2], which is directly connected to the H-He demixing. Functionals that take into account non-local correlations such as vdW-DF [3] are in better agreement with recent experiments [2]. Benchmarking studies with many XC functionals against QMC calculations suggest vdW-DF as an appropriate functional also for hydrogen-helium mixtures [4].
Here, we present a demixing phase diagram of H-He mixtures calculated with vdW-DF and compare with previous calculations derived with the PBE functional [5,6]. Differences and implications for planetary physics are discussed.

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[2] Knudson *et al.*, Science **348**, 1455 (2015).
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[6] Morales *et al.*, Phys. Rev. B **87**, 174105 (2013).

*E-mail address: manuel.schoettler@uni-rostock.de

The possibilities of proton radiography for the strongly coupled plasma EOS measurements

V.B. Mintsev*

Institute of Problems of Chemical Physics Russia Academy of Science, 142432, Chernogolovka, Moscow region, Pr. Semenova 1, Russia

In the present report possibilities of the proton radiography for equation of state measurements of shock compressed strongly coupled plasma of noble gases are discussed. We will analyze experiments with the shock-induced strongly coupled plasma of argon and xenon, which were conducted at the TWAC-ITEP proton radiography facility. The shock pressure P in argon tests was from 100 to 1000 bars, temperature T was 8-20 kK with non-ideality parameter Γ of about 1. In similar tests with xenon the values of P=4-6.5 kbar, T= 20-25 kK and Γ=1-2.5 were reached. The existence of shock waves in argon was registered by proton radiography. However the observed density gradient in these waves is of the same order as the sensitivity of the technique, so the accuracy of the experiment proved to be low. Considerably better situation is observed in xenon, where the formation and development of a shock wave and a plasma plug behind its front is firmly registered. Further processing of these proton radiography data on xenon allow to determine with sufficient accuracy the density of the developed strongly coupled plasma of xenon.

* email: minvb@ icp.ac.ru

Ionic transport through hydrophobic nanopores: theory and experiments

Manoel Manghi[*1], **Bastien Loubet**[1], **John Palmeri**[2]
[1] *Theoretical Physics Laboratory, Toulouse III Paul Sabatier University, Toulouse, France*
[2] *Charles Coulomb Laboratory, Montpellier University, Montpellier, France.*

Fundamental understanding of ionic transport at the nanoscale is essential for developing biosensors based on nanopore technology and new generation high-performance nanofiltration membranes for separation and purification applications.

We develop a mesoscopic theoretical approach for the electrolyte conductivity inside nanopores for various reservoir ionic concentrations. The model couples two types of approaches. A variational field-theoretic theory [1-2] allows us to describe the distribution of ions in the nanopore by including both dielectric exclusion and ion-ion correlation. In particular an 'ionic capillary evaporation' is predicted at low reservoir concentrations. Combined to the linear response theory, we then compute the various flux of ions, water and charges, through the nanopore.

The theory is then compared to experimental measurements of ionic transport through single putatively neutral hydrophobic nanopores made in polyethylene membranes [3] and through single-walled carbon nanotubes [4].
By fitting the experimental conductance data we show that additional effects such as advection by electro-osmotic flow, flow slip at the pore surface, surface charge regulation and local energy barriers along the tube, must be taken into account.

Contact : manghi@irsamc.ups-tlse.fr

[1] S. Buyukdagli, M. Manghi, J. Palmeri, *Phys. Rev. Lett.* **105**, 158103 (2010); J. Chem. Phys. **134**, 074706 (2011)
[2] B. Loubet, M. Manghi, J. Palmeri, J. Chem. Phys. **145**, 044107 (2016)
[3] S. Balme, F. Picaud, M. Manghi *et al.*, Scientific Reports **5**, 10135 (2015)
[4] K. Yazda *et al.*, submitted (2017)

The role of Coulomb correlations in nano-composite materials with high-*k* inclusions

Elshad Allahyarov[*1,2], **Hartmut Löwen**[2]

[1] *Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine Universität Düsseldorf, Universitätstrasse 1, 40225 Düsseldorf, Germany*
[2] *Theoretical Department, Joint Institute for High Temperatures, Russian Academy of Sciences (IVTAN), 13/19 Izhorskaya street, Moscow 125412, Russia*

Mixing dielectric polymers with high-*k* inclusions can affect their electrical properties. In actuation applications of dielectric elastomers, the polarized inclusions generate additional volume polarization-related electrostriction. In energy storage applications, it is possible to store more energy in dielectric composites because of additional polarization of the inclusions and interfaces. However, mixing electroactive polymer with high-*k* inclusions also brings several disadvantages. The expulsion of the field from the interior of high-k fillers and the presence of two poles on the filler surface along the applied field direction result in higher local fields E_L near the inclusion poles. The resulting field enhancement lowers the breakdown field (E_b) threshold for the material and therefore compromises the actuation and energy storage capabilities of dielectric composites. To mitigate this issue, the dependence of E_L on the morphology of inclusion distribution, the field localization effect in chained configurations, and the role of the dipole-dipole *correlation effects* in the enhancement of the dipolar field of inclusions are analyzed. We show that the dipolar *correlation effects* are strong in large inclusion composites and their contribution to the inclusion dipole moment μ and to the local fields E_L can reach 30-50 %. A new method for deriving the composite permittivity from the field E_L distribution, based on a caged probe technique, is also presented.

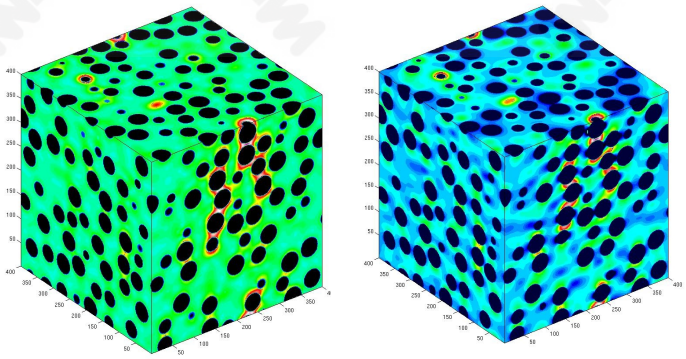

Figure: *3D distribution of the local field E_L/E_o (left picture) and its z-component E_z/E_o (right picture) in a dielectric elastomer composite with packing fraction of inclusions η=0.3. High fields are localized in chained particle configurations along the applied field E_o. The system parameters are: E_o=50 MV/m, ε_1=3 (the matrix),ε_2=1000 (the inclusions), σ=100nm.*

[1] E. Allahyarov et al, Smart Materials and Structures 23, 115004 (2014).
[2] E. Allahyarov et al, J. Appl. Phys. 117, 034504 (2015).
[3] E. Allahyarov et al, Phys. Chem. Chem. Phys. 17, 32479 (2015).
[4] E. Allahyarov et al, Phys. Chem. Chem. Phys. 18, 19103 (2016).

* email: elshad.allakhyarov@case.edu

Experiments and simulations on dusty plasmas

Yan FENG[*1], **Dong HUANG**[1], **Wei LIN**[1], **Wei LI**[1]

[1] *College of Physics, Optoelectronics & Energy, Soochow University, Suzhou, China*

Laboratory dusty plasma consists of micron-sized particles of solid matter, or dust particles, immersed in a plasma of free electrons and ions. These dust particles gain a large electric charge, typically ~-10^3e, so that they become strongly coupled. Due to its suitable time and length scales, the motion of individual particle can be directly imaged and tracked using video microscopy. Because of the shielding effects of free electrons and ions, these dust particles interact with each other through the Yukawa potential. In the past two decades, an abundance of dusty plasma experiments have been performed, including 1D, 2D and 3D suspensions of dust particles. Two types simulations of Yukawa liquids and solids have been widely used to study strongly coupled dusty plasmas, one is the frictionless equilibrium molecular dynamical (MD) simulation, the other is the Lengevin dynamical simulation.

Here, from frictionless equilibrium MD simulations, we have obtained a concise equation of state (EOS) for 2D liquid dusty plasmas [1-3]. This EOS contains three important physical quantities of dusty plasmas, the internal pressure, the coulping parameter, and the screening parameter. From this EOS, different thermodynamical processes can be analytically derived, such as isotherms, isobars, and isochores [2]. Also, various physical properties of 2D liquid dusty plasmas can be derived directly, like the bulk modulus of elasticity [4], as shown in Fig. 1. Using this bulk modulus of elasticity, we have predicted the sound speeds in different conditions [4], which agree well with previous studies using completely different approaches, as shown in Fig. 2.

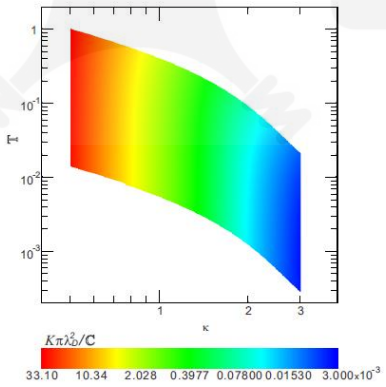

Figure1: *Bulk modulus of elasticity K for 2D liquid dusty plasmas*

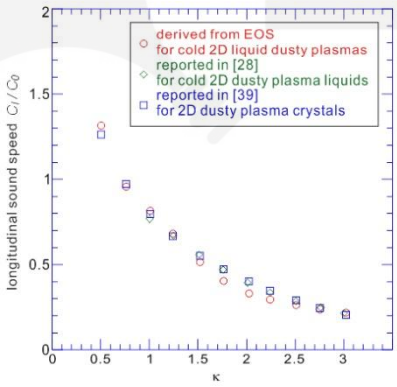

Figure2: *Comparison of sound speeds of 2D liquid dusty plasmas obtained from various methods*

[1] Y. Feng, J. Goree, B. Liu, L. Wang, and W.-D. Tian, J. Phys D: Appl. Phys. **49**, 235203 (2016)
[2] Y. Feng, W. Lin, W. Li, and Q. Wang, Phys. Plasmas **23**, 093705; 119904 (2016)
[3] Y. Feng, W. Li, Q. Wang, and W. Lin, Phys. Plasmas **23**, 113705 (2016)
[4] W. Li, W. Lin, and Y. Feng, Phys. Plasmas **24**, 043702 (2017)

* email: fengyan@suda.edu.cn

Transport Properties of a Disordered 2D Complex Plasma Crystal

E Kostadinova[*1], **K Busse**[1], **N Ellis**[1], **C Liaw**[1], **L S Matthews**[1] **and T W Hyde**[1]

[1] *Center for Astrophysics, Space Physics & Engineering Research (CASPER), Baylor University, Waco, Texas, USA*

In condensed matter, a crystal without impurities at zero temperature acts like a perfect conductor for a travelling electron. As the amount of lattice disorder reaches a critical value, the electron wavefunction experiences a transition from an extended to a localized state – this is called Anderson localization. The existence of such transitions in 2D materials has been the subject of heated debate over the past few decades due to a disagreement between theoretical prediction and experimental observation.

In this work, we investigate the transport properties of the dusty plasma crystal by analyzing the diffusion of coplanar lattice waves travelling within the medium. This is accomplished by comparing numerical simulation results to the predictions of a novel mathematical method, called the spectral approach to delocalization. This technique determines (with probability 1) the existence of extended states in infinite disordered lattices of any dimension without the use of boundary conditions or scaling. Thus, a comparison between theoretical and numerical results may be used to evaluate the effect of physical boundaries and system size. This, in turn, allows the interplay between disorder-driven behavior and interparticle interaction in a strongly coupled dusty plasma system to be examined. Since complex plasma crystals exhibit characteristic distance and time scales which are easily observable by video microscopy, they should prove an excellent macroscopic analogue of a disordered 2D material for the study of localization phenomena in the classical regime.

Finally, the question of whether Anderson localization can be *experimentally observed* in a 2D complex plasma crystal will be examined. If so, this would allow direct determination of the manner in which spatial defects influence the dynamical behavior of such strongly coupled Coulomb systems.

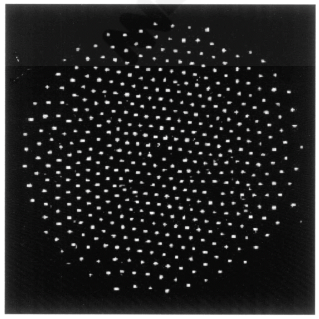

Figure: *Example of a single-layer complex plasma crystal* [1].

[1] G. A. Hebner, M. E. Riley, D. S. Johnson, P. Ho, and R. J. Buss, "Direct Determination of Particle-Particle Interactions in a 2D Plasma Dust Crystal," *Phys. Rev. Lett.*, vol. 87, no. 23, p. 235001, Nov. 2001.

* email: eva_kostadinova@baylor.edu

Critical and non-Critical Fluctuations in Mixtures of Ionic Liquids with Alcohols in the Vicinity of the Liquid-Liquid Phase Transition

Wolffram Schröer[*1], Bernd Rathke[2] , Alessandro Triolo[3], Olga Russina[4]

[1] Fb 2 Biologie-Chemie Universität Bremen, Bremen,Germany
[2] Technische Thermodynamik, Universität Bremen, Bremen, Germany
[3] Instituto Struttura della Materia, Consiglio Nazionale delle Ricerche, Rome, Italy
[4] Dipartimento di Chimica, Università di Roma Sapienza, Rome, Italy

Mesoscopic heterogeneities in binary mixtures of the ionic liquid ethyl-ammonium nitrate (EAN) with alcohols (pentanol and heptanol) are investigated by Small Angle X-ray Scattering as function of concentration and temperature ranging from 193 to 313 K. Such systems in general show a liquid-liquid phase transition which is driven by Coulomb interactions but modified by hydrogen bonding. Though macroscopically homogeneous, the mixtures are heterogeneous at the mesoscopic spatial scales. Two different heterogeneities are present: Critical concentration fluctuations centred at scattering vector Q=0, well known as precursors of the liquid-liquid phase transition e.g. for EAN/Octanol mixtures [1], and heterogeneities caused by segregation into ionic and non-ionic regions. The latter ones were predicted by simulation [2] and verified experimentally [3] in ionic liquids containing cations with long hydrocarbon chains. In pure EAN such structuring is observed as well giving rise to a band centred near Q = 6 nm^{-1} [4]. A similar band at Q =5 nm^{-1} is also observed in alcohols, again suggesting a segregation into polar and no-polar regions as a special case of charge ordering. Those heterogeneity bands of EAN and alcohols merge in mixtures. When approaching the critical composition and lowering the temperature towards the critical temperature, critical concentration fluctuations dominate and overshadow the ionic-non-ionic heterogeneity band. A careful analysis shows that this band reveals but is shifted towards small figures of the scattering vector. The Q=0 band varies with concentration, temperature and Q as expected for critical fluctuations. For the system EAN / heptanol the phase diagram was measured with an upper critical solution point at 259K and a critical composition at x= 0,64. In the case of the pentanol system [5] the critical solution point is virtual as it lays inside the solid phase region and thus cannot be reached in the experiment. For this system the critical temperature is estimated by extrapolation to Tc≈190 K. A pseudo spinodal is constructed applying the scaling laws of critical fluctuations .

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[*] email: schroer@uni-bremen.de

Quantum-Gas Microscopes – Quantum Simulation with Single-Particle Access

Stefan Kuhr *[1]

[1] *University of Strathclyde, Department of Physics, Glasgow, UK*

Trapping ultracold atoms in well-controlled engineered environments in optical lattices has proved to be a powerful tool for quantum simulation of strongly correlated quantum systems. The great challenge to obtain full single-site resolution and single-atom control in optical lattices was overcome by the development of quantum-gas microscopes [1,2]. In my talk I will give an overview of the recent developments in this field including our recent results on realizing single-site- and single-atom-resolved florescence imaging of fermionic ^{40}K atoms using electromagnetically-induced-transparency cooling [3]. Fluorescence imaging of atoms has made it possible to directly observe bosonic and fermionic many-body quantum systems with single-atom resolution in an unprecedented way, giving access to, e.g., in-situ measurements of temperature and entropy distributions, direct observation of correlations and their spreading, or the build-up of entanglement.

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* email: stefan.kuhr@strath.ac.uk

Ab initio simulations of the transport of strongly correlated fermions

Niclas Schlünzen[*1], **Jan-Philip Joost**[1], **Michael Bonitz**[1]

[1] *Institut für Theoretische Physik und Astrophysik, Christian-Albrechts Universität, Kiel, Germany*

The nonequilibrium dynamics of correlated fermions in lattice systems are of high current interest in the communities of both condensed matter and ultracold atoms. While there is a very fruitful progress in present experiments (e.g. Ref. [1]), the theoretical description constitutes a challenging task, especially in the regime of strong coupling and higher dimensions.

In this talk, I will introduce a description of correlated fermions in the framework of the nonequilibrium Green functions (NEGF) theory [2] which can be used to close this theoretical gap. I will demonstrate the accuracy and reach of the NEGF method by comparing the results to exact diagonalization, the density matrix renormalization group (DMRG) technique [3], as well as to two-dimensional experiments with ultracold atoms [4].

Finally, the NEGF method gives access not only to the single-particle density matrix, but also to two-time quantities (double occupation, pair correlation function, entanglement entropy) as well as to the time-dependent and spatially resolved spectral function and dispersion relation, where the correct description of correlations plays a crucial role.

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* email: schluenzen@theo-physik.uni-kiel.de

Simulation of stopping power and evolution of ion temperature in plasmas

Bin He *, **Wu Yong, Jun-Wen Gao and Jian-Guo Wang**

Institute of Applied Physics and Computational Mathematics, Beijing 100088, P.R. China
*Corresponding author: Hebin-rc@163.com, Wu-yong@iapcm.ac.cn

Stopping power for (SP) ions in warm dense plasmas is relevant to the research of fundamental plasma physics such as the transportation and inelastic transition in dense plasmas, which has potential application in controlled nuclear fusion. *Ab initio* research of SP is important to know more physics behind it and the design of fusion target. Here first we will introduce our recent work in this field [1-2], where all the related important mechanisms including the contribution of plasma polarization and inelastic transitions are considered in *ab initio* way. Our results [2] are found in good agreement with the experimental data [3] in both cool and warm matters at solid density. For solid material or condense matter at room temperature a new physical scenario is proposed to get SP at high projectile velocity [4]. Our work can explain why the usual local density approximation does not agree well with the experiment in cool matter. Non Fermi-Dirac distribution of free electron velocity is obtained self consistently, which may have influence upon the basic property of dense plasmas. Some predictions of SP are suggested which we hope to be tested in future in order to judge the existence of the new velocity distribution in dense plasmas, which become more apparent in strongly coupled plasmas.

Ultra-cold neutral plasmas can be produced in a magneto-optical trap where the ion temperature may be as low as about 1K. Such plasmas are helpful to research strong coupled system and in China relevant experiments are being progressed. In recent year we have made some classical molecular dynamical simulations about the evolution of the ion temperature in such plasmas [5], which we will introduce here. In the simulation all the Coulomb interactions among charged particles are adopted and Verlet-algorithm method has been used to get the positions and velocities of charged particles in its evolution processes. About 6000 ions and 6000 electrons are simulated where their mass ratio is 1000, and both Gaussian and ordered initial position distributions are considered. While disorder-induced heating is absent in the initially ordered distributions, the ions are found heated mainly by electron-ion collisions. The value of the strong coupling parameter is found to typically fall below 10 for realistic plasma densities.

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Constructing the free energy of finite-temperature spin-polarized electron liquids from quantum many-body theories

Shigenori Tanaka[*1]

[1] *Graduate School of System Informatics, Kobe University, Kobe 657-8501, Japan*

Theoretical approaches to accurately expressing the free energy or the equation of state for finite-temperature, spin-polarized, uniform electron fluid (gas or liquid) as the functions of density, temperature and spin polarization (ζ) are reviewed. The calculations of interaction energy and exchange-correlation free energy are performed in a compact form in the case of random-phase approximation (RPA). The strong-coupling effects beyond the RPA are then taken into account by the local-field correction (LFC) in the framework of dielectric response formalism [1]. The LFC has been well described in terms of various schemes such as the Singwi-Tosi-Land-Sjolander (STLS) [1-4], convolution (CA) [5], and hypernetted-chain (HNC) [6] approximations. We have carried out these analytical studies and compared the calculated results for the correlation and thermodynamic functions. We have then constructed the fitting formulae for the exchange-correlation free energy as the functions of r_s, θ and ζ in the cases of STLS [2,3], its improved version (iSTLS) [1,4], modified CA (MCA) [5] and HNC [6], which have also been compared with recent quantum Monte Carlo (QMC) based results [7,8], as shown in the figures below.

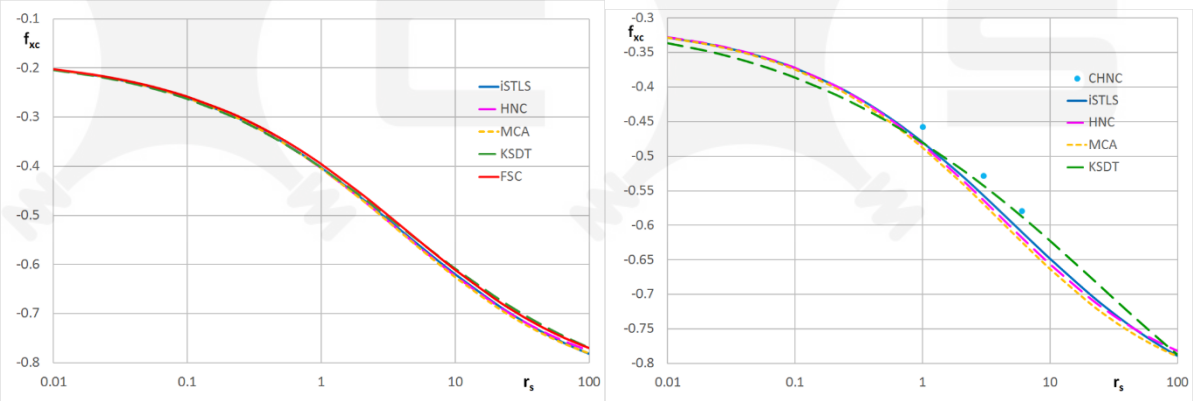

Figure: *Exchange-correlation free energies as functions of r_s at θ = 1 in the paramagnetic (left) and ferromagnetic (right) states [4]. KSDT and FSC refer to the QMC results in [7] and [8], respectively.*

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* email: tanaka2@kobe-u.ac.jp

Energy relaxation in warm dense matter

Jan Vorberger*

Institute of Radiation Physics, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

The interaction of lasers, particle beams or shock waves with matter generates non-equilibrium states due to the high energy intake over a very short time. Lasers mostly interact with the electrons. Particle beams couple either to electrons or ions, depending on their energy, respectively. Shock waves only heat the heavy particles. Therefore, systems are created in which one species of particles has a significantly higher energy than the others. The theoretical description of the relaxation of such states towards a (new) equilibrium poses considerable difficulties and the experimental investigations remain very challenging [1], all while applications in materials science, inertial fusion, and warm dense matter experiments become more important.
This talk covers recent developments in theory and experiment of energy relaxation processes from the realization of the importance of coupled mode effects for the energy transfer [2], to the relation between temperature and energy relaxation in correlated quantum systems [3], and to the limits of the standard two-temperature model [4]. Today, a combination high energy optical lasers, x-ray lasers, and x-ray scattering diagnostics allows to create and diagnose non-equilibrium states at the transition from high pressure solids to warm dense matter. Therefore, an overview of challenges, unsolved problems and available methods for such systems is given. This includes the theory for the non-equilibrium structure needed to understand the x-ray scattering signal as well as theory for the energy transfer in a highly correlated system.

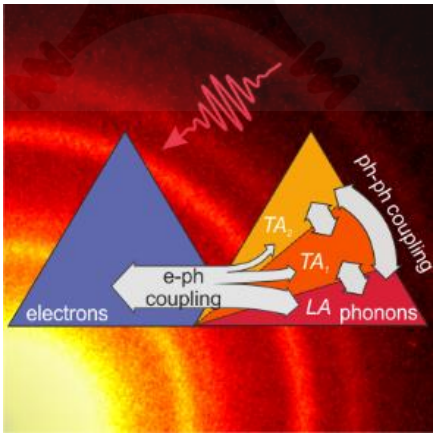

Figure: Schematic view of the mechanism of electron-phonon coupling in laser heated aluminium [4].

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* email: j.vorberger@hzdr.de

Interplay between quantum electrons and coupled ions: ion-electron temperature relaxation in dense hydrogen

Qian Ma, Jiayu Dai*, Dongdong Kang, Zengxiu Zhao, Jianmin Yuan

Department of Physics, College of Science, National University of Defense Technology, Changsha, Hunan 410073, P. R. China

The electron-ion temperature relaxation is an important non-equilibrium process in warm and hot dense matter and the Coulomb interaction is dominated in the scaterring process. In the strongly coupled regime, the electronic quantum effects may play an important role in the scattering process. Molecular dynamics (MD) [1] is considered as an effective method to investigate temperature relaxation. Here we use an electron force field (eFF) [2,3] method based on MD considering the electronic quantum effects to investigate the temperature relaxation processes in which electrons are considered as Gaussian wave packets while nuclei are still considered as charged points. The results show that electronic quantum effects extremely decrease the energy exchange rates and may influence the final thermal properties. The temporal evolution of ion-electron temperatures is shown in Fig.1 and the results of eFF and classical MD are compared [4].

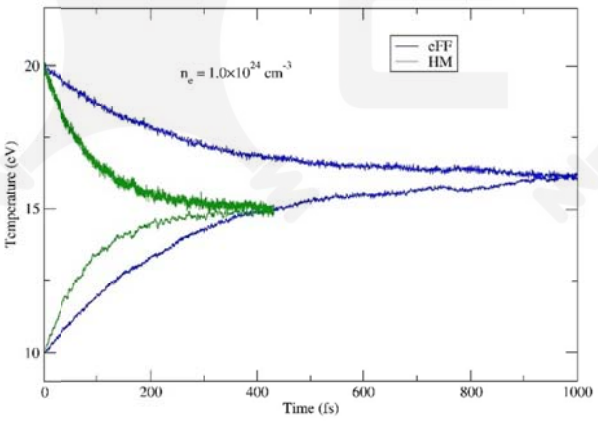

Fig.1:The temporal evolution of ion-electron temperatures. The blue lines represent eFF method and the green lines represent classical MD with HM potential. In the process, the electron temperature is higher than ion temperature.

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* email: jydai@nudt.edu.cn

Ionization potential depression in terms of the dynamical structure factor

Chengliang Lin[*1], **Heidi Reinholz**[1], **Gerd Röpke**[1], **Wolf-Dietrich Kraeft**[1]

[1] *Institut für Physik, Universität Rostock, 18051 Rostock, Germany*

The modification of the ionization potential due to a plasma environment, known as ionization potential depression (IPD), is of essential importance in determining the thermodynamic properties and optical properties of plasmas. Contrary to the commonly used analytical approaches [1, 2], we take into account the ionic correlation effect by introducing the dynamical structure factor within the framework of the quantum statistical theory. A general expression for the IPD is obtained [3]. Comparisons with other theories and different experimental measurements [4, 5, 6] are shown. For the later, good agreements are found. In particular, for mixtures with large mass and charge asymmetry, where the experimental results can not be explained by the widely used models so far, our approach is demonstrated to be valid.

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* email: chengliang.lin@uni-rostock.de

EQUATION OF STATE AND TRANSPORT PROPERTIES OF METALS IN WARM DENSE MATTER REGIME

Khomkin A.L., Shumikhin A.S.*
Joint Institute for High Temperatures of the Russian Academy of Sciences, Moscow, Russia

Measurements [1, 2] of plasma electrical conductivity were carried out in wide range of densities for temperatures above the critical for various metals (Al, Fe, Ni, Cu). This state called warm dense matter (WDM) or supercritical fluid (SCF). These measurements demonstrated continuous transition from gas-plasma to metal conductivity at density increase. In the most of offered theories [3, 4] the emergence of metal conductivity is explained by abnormal influence of Coulomb nonideality ($\Gamma \sim 100$) which leads to two or three multiple ionization of metal atoms already at $T = 10000$ K and provides thereby high, but gas-plasma conductivity. But, the equation of state was not calculated in this studies because of abnormal Coulomb nonideality turns to absurdity in pressure calculation.
In this study, we offer generalization of the model [5] for the accounting of processes of thermal ionization. The offered Helmholtz free energy for dense metal vapors describes mixture of the atoms connected by the electron jellium and also nonideal free ions and electrons. Jellium electrons, arise on tails of wave functions of valence electrons and exist at negative energy, and free, thermal electrons, at positive energy and they coexist independently. We put forward the statement that the electron jellium is present in atomic gas at any density. Reason trivial: the isolated atom occupies the entire space, and in ensemble of other atoms a volume, restricted the Wigner-Seitz radius. Concentration of electrons of jellium was determined by various ways. Concentration of thermal electrons was determined by the Saha formula taking into account all considering types of correlations. The calculations of conductivity show a satisfactory agreement with experiments [1, 2] and describe continuous transition from gas-plasma conductivity (thermal electrons, small density) to metal conductivity (jellium electrons, high density). The equation of state is calculated for expanded metals also. The obtained results are in good agreement with experimental data and numerical simulation (QMD) [1, 2].

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*e-mail: shum_ac@mail.ru

Influence of the ionization on ionic transport properties in the warm dense regime

Yong Hou[1,+], Jiayu Dai, Dongdong Kang[1], and Jianmin Yuan[1,2,++]

1*Department of Physics, College of Science, National University of Defense Technology, Changsha 410073, People's Republic of China;*
2*Graduate School, China Academy of Engineering Physics, Building 9, Zpark II, 100193 Beijing, People's Repubic of China.*

In the warm dense regime, transport properties are the crucial input parameters in hydrodynamic simulations. However, it is difficult to describe the ionic and electronic structures because all physical ingredients, such as coulomb interactions, pressure ionizations, electron degeneracy and ion-ion strong coupling, must be taken into account. In particular, ionic physical properties are influenced by these effects. Here, we perform average-atom molecular dynamics (AAMD) to simulate the CH and LiH mixtures and compute the equation of state and ionic transport properties. In the AAMD model, electronic structures are calculated by using the modified average-atom model, which have included the broadening of the energy levels, and the ion-ion pair potentials of mixtures are constructed based on the temperature-dependent density functional theory. The ionic transport properties, such as ionic diffusion and shear viscosity, are obtained through the ionic velocity correlation functions. Through comparing the results, it is shown that transport properties depend not only on the ionic mass but also on the average ionization degree.

+yonghou@nudt.edu.cn;
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Phase transitions in spin-orbit coupled systems

Gordon Baym[1]

[1] *Department of Physics, University of Illinois, Urbana, IL 61801, U.S.A.*

Spin-orbit coupling occurs naturally in electronic systems and can also be simulated in cold atomic gases [1]. This talk will focus primarily on the cold atom gases where one has remarkable control over the atomic species, density, and interactions among the constituents. At zero temperaure bosonic cold atom systems exhibit a rich phase structure, with quantum phase transitions between plane-wave condensates, striped condensates, and an unstable phases [2]. At finite temperature the transition from condensed to normal, for pure Rashba coupling, is first order in mean field theory [3], but more likely second order with fluctuations taken into account [4]. Spin-orbit coupling has the further effect in fermionic cold atoms of modifying the evolution from Bardeen-Cooper-Schrieffer pairing to Bose-Einstein condensation, as well as the phase transition from normal to superfluidity [5].

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Excitonic condensation and quadriexcitons in a symmetric electron-hole bilayer with valley degeneracy: QMC simulations.

Gaetano Senatore[1*1], F. Tramonto[1], S. De Palo[2,1], S. Moroni[2,3]

[1]Dipartimento di Fisica, Universita` di Trieste, strada Costiera 11, 34151 Trieste, Italy
[2]CNR-IOM DEMOCRITOS, Istituto Officina dei Materiali
[3]SISSA Scuola Internazionale Superiore di Studi Avanzati, Via Bonomea 265, I-34136 Trieste, Italy

The realization of systems of spatially separated electrons and holes, in the search of the equilibrium excitonic condensate foreseen by [1], has gone on for more than two decades, but so far the condensate has eluded experimental detection [2]. It has been recently suggested that a substantial enhancement of the electron-hole attraction, to favour the condensate, could be obtained in coupled graphene bilayers [3]; a couple of experimental realizations has promptly followed [4]. Such systems have a quadratic energy dispersion on a wide density range and a twofold valley degeneracy in each bilayer.
We have embarked in extensive QMC simulations of an electron-hole bilayer with mass symmetry and twofold valley degeneracy (in each layer), to partially mimic the situation encountered in the coupled graphene bilayers proposed in [2]. Our goal is to provide benchmark results for the electron-hole bilayer investigating the qualitative and quantitative effects of the valley degeneracy, inferred by comparison with the conventional electron-hole bilayer possessing only spin degeneracy [5].
We have studied systems of 168 particles, for in-layer densities corresponding to $1 \le r_s \le 8$ and inter-layer distances $1 \le d/a_B \le 4$. We find an excitonic condensate for $r_s \gtrsim 1$ at intermediate distances, whereas a quadriexciton fluid [6] and a plasma fluid are stable respectively at smaller and larger distances. The region of stability of the excitonic condensate is significantly shrunk with respect to the system without valley degeneracy [5]. Moreover we observe for the first time the formation of quadriexcitons, first predicted by Wang and Kittel [6] 45 years ago.

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* email: senatore@units.it

Strongly correlated electron-hole 2D systems: current status and perspectives

Yu.E. Lozovik[*1]

[1]*Institute of Spectroscopy RAS, 142190, Troitsk, Moscow, Russia*

Electron-hole bilayers based on semiconductor nanostructures, graphene and topological insulators, superfluidity and strongly correlated states will be reviewed. (see also [1-9]). Role of the hybridization will be analyzed.

Drag effect , Cooper electron-hole pair fluctuations and fluctuational internal Josephson effect in the system will be considered.

Anisotropic superfluidity, instabilities and strong correlated phases in dipole systems will be analyzed. Anisotrpies of helicity modulus, superfluid mass density, speed of sound and quasicondensate luminiscence are predicted for a two-dimensional system of interacting dipole excitons in a periodic potential at $T = 0$. Presence of supersolid properties in the system considered is shown. Physical realizations of the model are discussed. For a system of two-dimensional dipolar excitons in an electrostatic lattice estimates for the magnitude of the predicted effects are given and a method to control superfluid component and measure helicity modulus in dipolar systems is presented. Roton instability of dipole exciton system in semiconductor film is discussed.

Strong correlated phases of dipole excitons (or dipole atoms) will be discussed. Experimental manifestation of the predicted effects will be analyzed.

Instabilities in the system of dipole excitons (excitons with spatially separated electron and holes) will be analyzed.

Possible crystal and supersolid phases in dipole exciton systems will be discussed. The transition of the exciton system from the superfluid state to a non-superfluid state controlled by gate and its manifestation by light scattering will be analyzed.

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* email:lozovik@isan.troitsk.ru

Charge Density Waves in the Electron-Hole Liquid in the Coupled Quantum Wells

Polishchuk I.Ya.[*1,2], **Babichenko V.S.**[2]

[1] *National Research Center Kurchatov Institute, Moscow, 123182, Russia*
[2] *Moscow Institute of Physics and Technology, Dolgoprudnii, Russia*

For the first time the electron-hole plasma (EHP) in the coupled quantum wells (CQW) where the electrons and the holes a spatially separated was studied in [1]. Then, a possibility of the exciton Bose-Einstein condensation, the superfluidity, the superconductivity, the gas-liquid transition, Wigner crystallization etc. were investigated in various papers. Since the publication of paper [2], it was recognized that the *many-components* EHP in the *bulk* revealed the unconventional Coulomb screening. Such remarkable feature has motivated us to study the many-component spatially separated EHP in the CQW [3-6]. It was found that the homogeneous in-plane charge distribution is thermodynamically unstable for low-enough charge concentration, resulting in the appearance of electron-hole liquid drops [3]. The trend to formation of the EHL in such systems enhances if the difference between the electron- and the hole effectives masses is taken into account [4]. The thermodynamic instability is found to be induced by the instability of the one of the branch of the electron-hole excitation spectrum which is inherent specifically to the many-component EHP [5]. The quantum phase transition in the EHL is discovered in Ref. [6] which results in the creation of the charge-density waves (CDW). Correlations in electron-hole layers that result in a transition from the homogeneous liquid to a charge density wave are considered in Refs. [7, 8].

In the present contribution it is shown that the CDW appears due to the *plasmon* instability the EHL (the plasmon branch is quite the different one from that resulting in the appearance of the EHL itself [5]). This instability results in the appearance the in-plane charge distribution which is a honeycomb periodical lettice.

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* email: iyppolishchuk@gmail.com

Time-dependent calculation methods for studying the electronic dynamics of correlated systems

V.N. Valmispild[a,b*]; E. Gorelov[c]; M. Eckstein[d]; V. Antropov[e]; A. Lichtenstein[a,b,c]

[a]*Institute of Theoretical Physics, University of Hamburg, Jungiusstrasse 9, 20355 Hamburg, Germany*
[b]*The Hamburg Centre for Ultrafast Imaging, Luruper Chaussee 149, 22761 Hamburg, Germany*
[c]*European XFEL GmbH, Holzkoppel 4, 22869 Schenefeld, Germany*
[d]*Max Planck Institute for the Structure and Dynamics of Matter, 22761 Hamburg, Germany*
[e]*Ames Laboratory, Ames, IA 50011, USA*

The present work is focused on theoretical description of electron dynamics in correlated materials. The report consists of two sections:

1) Non-equilibrium dynamics of correlated materials: perturbation theory approach.
2) Magnetic susceptibility in transition metal systems.

In the first part we study the single-band Hubbard model in the presence of a large spatially uniform electric field. We study the Hubbard model out of equilibrium using the Keldysh formalism and perturbation theory in the Coulomb interaction U [1].

Using time dependent dynamical mean-field theory and perturbation theory we investigate the behavior of the photoemission spectra, total energy and double occupancy of the sites, as a function of time, and on-site Coulomb repulsion U. The calculations are performed on the Bethe lattice as a benchmark and on a two-dimensional square lattice.

In the second part we study dynamic magnetic susceptibility [2]. The spin-flip response function $\chi\pm$ is calculated by means of the Time Dependent Density-Functional Theory (TDDFT). We use the full-potential linearized augmented plane-wave method (FLAPW) implementation [3].
We calculate Magnetization [4] and the fluctuations of the magnetic moment for bcc-Fe, fcc-Co and fcc-Ni.

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* email: vvalmisp@physnet.uni-hamburg.de

Simulations of high intensity x-ray generated plasmas

Zoltan Jurek[*1,2], **Malik Muhammad Abdullah**[1,2,3], **Sang-Kil Son**[1,2], **Beata Ziaja**[1,2,4], **Robin Santra**[1,2,3]

[1] *Center for Free-Electron Laser Science, Deutsches Elektronen-Synchrotron, Hamburg, Germany*
[2] *The Hamburg Centre for Ultrafast Imaging, Hamburg, Germany*
[3] *Department of Physics, University of Hamburg, Hamburg, Germany*
[4] *Institute of Nuclear Physics, Polish Academy of Sciences, Krakow, Poland*

With the advent of the X-ray Free-Electron Lasers (XFELs) the experimental study of high energy density plasmas has become feasible. Within tens of femtoseconds even a single XFEL pulse can pump enormous energy into cold matter creating plasma out of it - on similar timescales. The cascading of x-ray induced inner shell electronic transitions as well as the plasma formation processes are complex non-equilibrium phenomena that require thorough theoretical investigations.

In this talk we present a simulation approach for studying the formation and the dynamics of high intensity x-ray generated plasmas. The framework includes the ab initio treatment of the atomic electronic structure and x-ray induced inner shell processes with the XATOM toolkit [1,3] and a hybrid Molecular Dynamics/Monte Carlo treatment of the mixture of the many atom/ion system and plasma electrons via the XMDYN code [2,3]. We outline the modeling concept and the capabilities of such a microscopic description. Further, we show comparisons between theoretical and experimental results towards the validation of the approach. Finally we discuss future perspectives.

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* email: zoltan.jurek@desy.de

Phase transitons in low-Z warm-dense-mater Carbon systems; NPA-DFT predictions of EOS, conductivity and XRTS spectra.

Chandre Dharma-wardana[*1]

1 *National Research Council of Canada, Ottawa, Canada. K1A 0R6.*

Standard Density-functional theory (DFT) calculations and molecular dynamics (MD) simulations show that low-Z elements like C, H, O, N etc., form transient chemical bonds even at temperatures as high as 8-10 eV. In fact the C=C double bond has an energy in that range. The study of these systems and their mixtures using DFT+MD, at higher temepratures is quite prohobitive, while low-T systems can be accessed. The calculated pair-distribution functions (PDFs) for WDM carbon by DFT+MD, and by the neutral-pseudo-atom (NPA) method show a first peak typical of the C-C bond length of such covalent bonding. The average-atom codes like PURGATORIO, MUZE, the model of Strarrett and Saumon, Blinski et. al. fail to capture these C -C bonding effects. They give PDFs typical of simple liquids, with no covalency peak. In contrast, the neutral-pseudo-atom (NPA) model based on a correlation sphere (CS) used by Perrot and the present author successfully recovers such bonding (see Fig) effects. The NPA-CS model reveals phase transitions in WDM carbon where the strongly correlated fluid undergoes a transition to un uncorrelated monoatomic liquid. The bonding in carbon requires 4 valence elctrons, and the phase transition is driven by a change in ionization which drops from 4 to ~3 at the phase transition, when C-C bonding is not possible. The EOS, transport properties, and the X-ray Thompson spectra (XRTS) of WDM-carbon across the phase tansition are presented. The possible existence of such phase transitions in other low-Z WDMs is of interest in astrophysics and ICF .

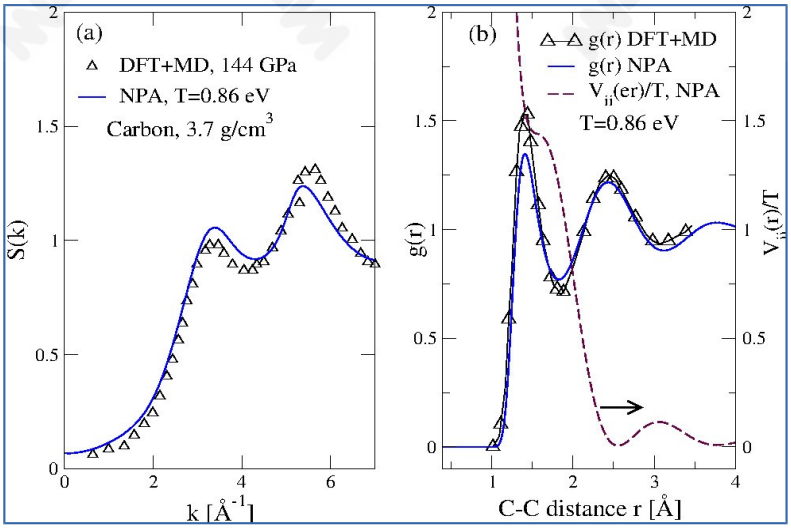

Figure: The Structture factor (left panel) of WDM carbon at 0.86 eV and 3.7 g/cc as calculated using DFT+MD, and using NPA. The right-hand panel gives the g(r), where the first-peak coresponds to a typical C-C covalent bonding distance. The usal average-atom codes fail to pick up bonding effects. The corerspondinfg pair-potential is also shown.

* email: chandre.dharma-wardana@nrc-cnrc.gc.ca [1] https://arxiv.org/pdf/1607.07511

Warm dense matter demonstrating non-Drude conductivity from observation of non-linear plasmon damping

B.B.L. Witte[*1,2], **L.B. Fletcher**[1], **E. Galtier**[1], **E. Gamboa**[1], **H.J. Lee**[1], **U. Zastrau**[3], **R. Redmer**[2], **S.H. Glenzer**[1], **and P. Sperling**[1,3]

[1] Universität Rostock, Institut für Physik, Rostock, Germany
[2] SLAC National Accelerator Laboratory, Menlo Park, USA
[3] European XFEL, Hamburg, Germany

X-ray Thomson scattering (XRTS) is an effective tool to determine plasma parameters, e.g., temperature and density, in the warm dense matter (WDM) regime [1]. Furthermore, transport coefficients are relevant for modeling, e.g., fusion experiments or the magnetic field generation in planets. Recently, the electrical conductivity was extracted for the first time from XRTS experiments on aluminum, isochorically heated by the Linac Coherent Light Source (LCLS) [2]. The measured spectrally resolved scattering signal shows a strong dependence on the electron interactions which has to be treated beyond perturbation theory.

We present simulations using finite-temperature density-functional-theory molecular-dynamics to calculate the dynamic thermal and electrical conductivity in warm dense aluminum. The comparison between exchange-correlation functionals in the PBE and HSE approximation indicates evident differences in the density of states and the dc conductivity. The HSE calculations show excellent agreement with experimental LCLS x-ray plasmon scattering spectra revealing a regime of damping below the Landau increment. These findings demonstrate non-Drude-like behavior of the dynamic conductivity that needs to be taken into account to determine the optical properties of WDM.

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* email: bastian.witte@uni-rostock.de

Quantum MD Simulations in Strong EM Fields

Hartmut Ruhl[*1], **Christian Herzing**[2]

[1] *Department of Physics, LMU, Munich, Germany*
[2] *LMU, Theresienstrasse 37, 80333 Munich, Germany*

Starting from first principles the physics of strong radiation fields interacting with electrons and positrons is revisited. With the help of a Wigner formulation of QED [1] and by arbitrarily splitting the radiation field into a classical and a quantum part a system of quantum molecular dynamical (QMD) equations of motion in strong electromagnetic fields with radiation reaction and spin is derived. For weak correlations semi-classical MD equations are obtained. For stronger correlations the quantum dynamical constraints lead to quantum event generators.The system of equations can be solved in order N operations with a grid free numerical algorithm, where N represents the number of particles [2].

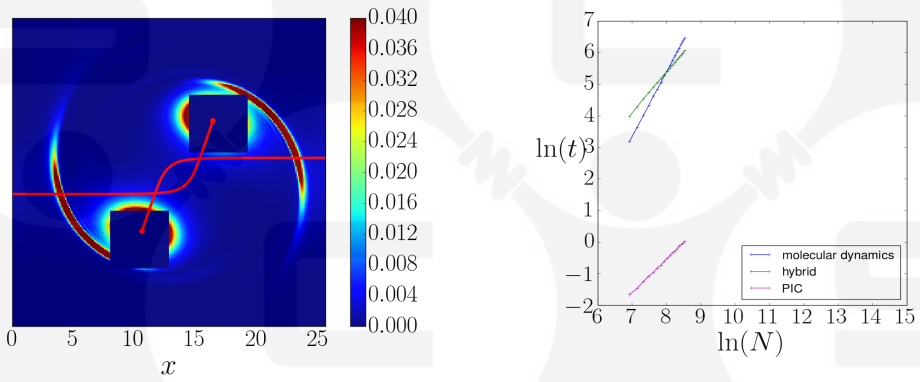

***Figure 1:** Electron-positron scattering with radiation (left) and scaling of the MD algorithm with particle number (right).*

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* email: hartmut.ruhl@lmu.de

Thomson scattering from dense non-equilibrium plamas

Th. Bornath[*1], **T.-N. Beuermann**[1], **C. Cordes**[1], **M. Shihab**[2], **R. Redmer**[1]

[1] *Institute of Physics, University of Rostock, Rostock, Germany*
[2] *Department of Physics, Tanta University, Tanta 31527, Egypt*

X-ray Thomson scattering (XRTS) experiments in the soft and hard X-ray regime yield information on fundamental parameters of high-density systems. Pump-probe experiments with variable time delay provide insight into the excitation and relaxation dynamics in dense plasmas on short time scales. Often, a theoretical description of states is applicable in which the electrons and ions are thermalized to different temperatures [1]. At even shorter time scales, states arise in which the electron distribution function (EDF) cannot be described by local equilibrium functions and a more detailed kinetic description is necessary.

There are different methods to calculate non-equilibrium properties, e.g., Monte Carlo (MC) simulations, particle-in-cell (PIC) simulations, hydrodynamics simulations, and kinetic equations. We have used all these methods in different contexts in order to provide some input of non-equlibrium properties into the calculation of synthetic Thomson scattering spectra.

We developed a MC code to calculate the EDF for the description of partially ionized hydrogen plasma droplets interacting with intense laser pulses in the XUV regime [2]. Recently, we studied the interaction of intense ultrashort laser pulses with cryogenic He jets using 2D3V relativistic PIC simulations [3]. Short pulses with intensities of 10^{16} W/cm^2 are found to drive ionization at warm dense matter conditions along the slab and outside the laser spot, the ionization front propagates along the slab at a considerable fraction of the speed of light. The temporal evolution of the ionization has been studied considering theoretically a pump–probe XRTS scheme.

Besides non-equilibrium effects on the EDF, there is a potential influence of spatial inhomogeneities on the scattering signal. The simplest approximation is to sum the contributions of the different volume elements assuming local equilibrium conditions [4]. Belyi [5] showed that the inclusion of gradients might have a great influence on the field and density fluctuations in a non-equilibrium plasma. While in [6] the density fluctuations have been studied, we present results considering both the field and density fluctuations.

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* email: thomas.bornath@uni-rostock.de

What is the correct choice of the plasma partition function and the lowering of the ionization energy - on contributions by Planck and Unsöld

Werner Ebeling
Institute of Physics, Humboldt University, Berlin, Germany

We analyze the contributions of scientists from Kiel, Max Planck and Albrecht Unsöld, to urgent questions of plasma physics [1,2,3].
Recently several workers question the regularized partition function proposed by Planck, Brillouin and Larkin (PBL) partition function and standard expressions for the lowering as given e.g by Unsöld. After reproducing the historical approaches
we explain the strict quantum-statistical foundation of the ionization theory [4]. Our view is based on Onsagers position in a famous historical controversy about the correctness of theoretical expressions for the mass - action constant of ion association. We explain why statements about correctness of regularized partition functions and bound energy lowering have no direct physical meaning. Applying Onsagers theorem we show that there is indeed some freedom in defining the partition function and the lowering, but in a complete theory this would not matter since according to Onsager, ``what we remove from one side of the ledger would be entered elsewhere with the same effect''.
In correct theories, which consider ``both sides of the ledger'',
the different choices of partition functions and the lowering may be used (in some limits) on equal rights. Finally we show that there is indeed an advantage
of the Planck - Brillouin - Larkin partition and a definite justification of the Unsöld expression for the lowering in certain density - temperature regions [4].

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Ultrafast probing of dense plasmas – visualizing dynamics of Strongly Coupled Coulomb Systems

S. H. Glenzer
SLAC National Accelerator Laboratory, 2575 Sand Hill Road, MS 19, Menlo Park, CA 94025. USA,

We have developed ultrafast scattering techniques to determine the physical properties of short-lived states of matter in extreme conditions. While X-ray Thomson scattering has been the technique of choice [1] to measure temperatures and densities in compressed dense plasmas [2] we have recently applied x-ray forward scattering on plasmons to determine collisions and conductivity [3,4]. These experiments utilize the Linac Coherent Light Source (LCLS), the world's brightest x-ray source that provides high repetition rate capability delivering data with unprecedented signal-to-noise levels. In parallel, new theories that go beyond the Chihara approximation and that use density functional theory in combination with the dissipation-fluctuation theorem are now available to interpret the scattering spectra. This novel approach provides new insights into the physics of strongly coupled Coulomb systems revealing non-Drude physics and non-linear plasmon damping effects. Future studies will apply these techniques to implosions on the National Ignition Facility where recent scattering measurements have demonstrated that this platform will approach nearly degenerate matter at ultrahigh densities (ρ = 40 g/cm^3; $n_e = 10^{25}$ cm^{-3}) [5,6]. In this talk, we will discuss these new studies and will provide an outlook for future developments in this area to develop our understanding of strongly coupled Coulomb systems through precision measurements of the dynamic structure factor.

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This work was supported by DOE Office of Science, Fusion Energy Science under FWP 100182. Part of this work was performed under the assistance of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 and by the Deutsche Forschungsgemeinschaft (DFG) within the SFB 652

*E-mail address: glenzer@slac.stanford.edu

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ACCELERATOR Driven High Energy Density Science
-Status of HED Physics at FAIR and GSI-

D.H.H. Hoffmann[1,2] on behalf of High Energy Density Physics Collaboration[3] at FAIR,
TU Darmstadt and National Research Nuclear University "MEPhI", Moscow"

[1]Technical University Darmstadt, Hessen, Germany
[2]National Research Nuclear University, Moscow Institute of

High intensity particle accelerators like FAIR at GSI Darmstadt and the proposed HIAF facility in China are a new tools to induce High Energy Density states in matter. Physics (HEDP) with intense heavy ion beams as a tool to induce extreme states of matter. The development of this field connects intimately to the advances in accelerator physics and technology. We will cover the generation of intense heavy ion beams starting from the ion source and follow the acceleration process and transport to the target. Intensity limitations and potential solutions to overcome these limitations are discussed. This is exemplified by citing examples from existing machines at the Gesell-schaft fu¨ r Schwerionenforschung (GSI-Darmstadt), the Institute of Theoretical and Experimental Physics in Moscow (ITEP-Moscow), and the Institute of Modern Physics (IMP-Lanzhou). Facilities under construction like the FAIR facility in Darmstadt and the High Intensity Accelerator
Facility (HIAF), proposed for China will be included. Developments elsewhere are covered where it seems appropriate along with a report of
recent results and achievements.
This research was supported by BMBF research grants: 05P12RDFN6; 05P12RDB7; 05P12RDBK; 05P12RDRBN and 05K10RD,
DFG-RFBR (German Science Foundation- Russian Foundation of Basic Research),
Russian grant of scientific school НШ - 5814.2014.2,
and China NSFC grants: U1532263, 11505248, 11375034, 11205225, 11275241, and 11275238

Ionization Measurements in 30-fold Compressed, Near-Degenerate Plasmas*

T. Doeppner,[1,†] D. Kraus,[2,#] P. Neumayer,[3] D.O. Gericke,[4] B. Bachmann,[1] R. Baggott,[4] D. Chapman,[5] G.W. Collins,[1] L. Divol,[1] R.W. Falcone,[2] L. Fletcher,[6] S.H. Glenzer,[6] A. Kritcher,[1] O.L. Landen,[1] M. MacDonald,[2] C. Mauche,[1] A. Pak,[1] R. Redmer,[7] A. Saunders,[2] P. Sperling,[6,9] C. Weber,[1] B. Witte,[6,7] and A. Yi[9]

[1]*Lawrence Livermore National Laboratory, Livermore, CA 94550, USA*
[2]*Department of Physics, University of California, Berkeley, CA 94720, USA*
[3]*GSI Helmholtzzentrum für Schwerionenforschung, 64291 Darmstadt, Germany*
[4]*Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom*
[5]*Plasma Physics Group, AWE plc, Reading RG7 4PR, United Kingdom*
[6]*SLAC National Accelerator Laboratory, Menlo Park, CA 94309, USA*
[7]*University of Rostock, Institute of Physics, 18051 Rostock, Germany*
[8]*European XFEL GmbH, 22869 Schenefeld, Germany*
[9]*Los Alamos National Laboratory, Los Alamos, NM 87545, USA*
[#]*current affiliation: Helmholtz Zentrum Dresden-Rossendorf, Germany*
†*doeppner1@llnl.gov*

Abstract. A precise knowledge of ionization at given temperature and density is required to accurately model compressibility and heat capacity of materials at extreme conditions. We have developed an experimental platform for x-ray Thomson scattering (XRTS) measurements at the National Ignition Facility [1-3] to characterize the plasma conditions in plastic and beryllium capsules in implosion experiments near stagnation. Recently, we have demonstrated XRTS measurements from capsules that were compressed to 30 g/cm^3 and inferred electron densities approaching 10^{25} cm^{-3}, corresponding to a Fermi energy of 170 eV and pressures exceeding 1 Gbar. We will discuss recent results, which show significantly higher ionization than predicted by widely-used ionization models like Stewart & Pyatt.

* This work was performed under the auspices of the US Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

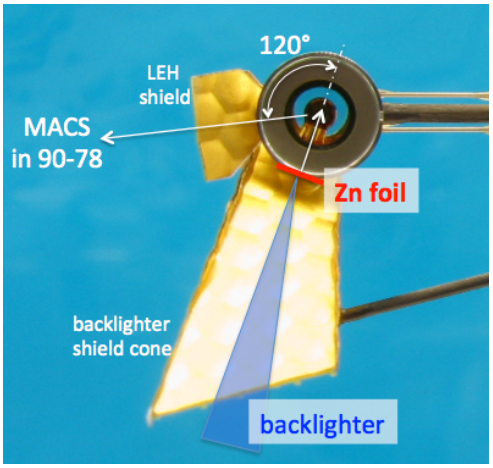

Figure: *Target platform for x-ray Thomson scattering measurement from capsule implosion experiments at the National Ignition Facility [2]. Zinc He-alpha x-rays (9 keV) scattering at 120 degree off the compressed capsule yield high sensitivity to K-shell ionization in beryllium and carbon, while at the same time constraining density and temperature.*

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Ionization of molecules at the fluid-fluid phase transition in warm dense hydrogen

Genri Norman*[1,2], Ilnur Saitov[1,2]

[1] National Research University Higher School of Economics (NRU HSE), Moscow, 101000, Russia
[2] Joint Institute for High Temperatures RAS, Moscow 125412, Russia

An idea is introduced that ionization of H_2 moleculas takes place at the fluid-fluid phase transition in warm dense hydrogen/deuterium (WDH) with formation of molecular ions H_2^+ and H_3^+. Ab initio molecular dynamics and density functional theory with the VASP plane-wave code are used. Proton-proton pair correlation functions (PCF) g(r), conductivity and pressure are calculated. The results are averaged over the set of equilibrium configurations. The approach is a conventional one. However, three PCF treatment procedures are applied to reveal a nature and character of the phase transition.

(1) PCF varies slowly with the density in the range of distances larger than 2Å. However, the situation changes drastically for distances smaller than 2Å. The values of the PCFs first local maxima $g(r_{max1})$ and first local minima $g(r_{min1})$ are changed dramatically in the narrow density range. To emphasize the character of g(r) changes, plots of $g(r_{max1})/ g(r_{min1})$ are obtained. Strongly pronounced jumps for T = 700, 1000, 1500 and 2500 K are clear indications of the phase transition since they take place at the same densities where small density jumps are observed.

(2) The value of r_{max1} is equal to the interatomic distance d_{H_2} = 0.74Å, in the H_2 molecule. The value of r_{min1} is close to the interatomic distances $d_{H_2^+}$ = 1.06Å, and $d_{H_3^+}$ = 0.92Å, in the molecular ions H_2^+ and H_3^+. Let $g_1(r)$ and $g_2(r)$ are PCF's which are the closest to the phase transition before and after it. It is shown that $\Delta g(r)= g_2(r)-g_1(r)$ is close to zero for r>2Å. The function Δg(r) has a deep minimum at $r= d_{H_2}$ and a strongly pronounced maximum in the range of r from $d_{H_3^+}$ to $d_{H_2^+}$. It means that the number of H_2 molecules decreases and molecular ions H_2^+ and H_3^+ appears at the phase transition.

(3) The ratio of the second maxima and minima $g(r_{max2})/ g(r_{min2})$ varies smoothly with the density. It turns out that the PCF's obtained can be modeled for r larger than 2Å, by the soft sphere PCF's at number densities which are equal to the total number density of H_2, H_2^+ and H_3^+. The latter value remains close to the constant one at the phase transition. The repulsion “diameters” is close to the theoretical estimate.

Strong ionization during the fluid-fluid phase transition in WDH distinguishes it from the Brazhkin-type liquid-liquid phase transitions. It can be related to the Norman-Starostin plasma phase transition prediction. However, it differs from it by inherent structural changes. The transition in WDH is an exceptional case.

The study has been funded by the Russian Academic Excellence Project '5-100'.

* email: genri.norman@gmail.com

Multicomponent electron-hole superfluidity and the BCS-BEC crossover in double bilayer graphene

Andrea Perali[1], **Sara Conti**[2,3], **Francois M. Peeters**[3], **David Neilson**[2,3]

[1] *School of Pharmacy, Physics Unit, University of Camerino, Italy*
[2] *School of Science and Technology, Physics Division, University of Camerino, Italy*
[3] *Department of Physics, University of Antwerp, Belgium*

The recent fabrication of two very close, but electrically isolated, conducting bilayer graphene sheets, one containing electrons and the other holes with tunable densities [1–3], raises exciting possibilities of observing high-temperature electron-hole superfluidity [4], since the electrons form pairs with the holes through very strong Coulomb attraction [5-6], which leads to large superfluid energy gaps [7].

Here we predict that superfluidity in coupled electron-hole sheets of bilayer graphene is multi-component because of the conduction and valence bands contributing to superfluidity [8]. We investigate the superfluid crossover properties as functions of the tunable carrier densities and the tunable energy band gap Eg separating the valence and the conduction bands. For small band gaps there is a significant boost in the two superfluid gaps, but the interaction driven excitations from the valence to the conduction band can weaken the superfluidity, even blocking the system from entering the BEC regime at low carrier densities. At a given larger density, a band gap Eg∼40-60 meV can carry the system into the strong-pairing multiband BCS-BEC crossover regime, the optimal range for realization of high-Tc superfluidity with sizable superfluid gaps.

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e-mail: andrea.perali@unicam.it

Coupled plasmon modes in vertically stacked 2D nanomaterials

E. H. Hwang* **and P. Park**

SKKU Advanced Institute of Nanotechnology, Sungkyunkwan University, Suwon 16419 Korea

We describe the diagrammatic formulation of the many-body theory for coupled interacting systems of different dimensions and materials. The formulation is applied to a one-dimensional quantum wire coupled to a two-dimensional electron gas and the vertically stacked 2D layers with an interlayer separation of d. Especially, we present the plasmon dispersion and its damping in vertically stacked graphene/MoS2 heterostructure with carrier densities n1 and n2, respectively. The linear chiral gapless single-particle energy dispersion of graphene leads to plasmon properties with several unexpected experimentally observable characteristic features such as a nontrivial influence of an undoped (n1=0) graphene layer on the coupled plasmon dispersion and a strange influence of the second (MoS2) layer even in the weak-coupling d→∞ limit. At long wavelengths (q→ 0), the density dependence of the coupled plasma frequencies is different from the usual 2D electron system with quadratic energy dispersion. We also investigate plasmonic properties of twisted-bilayer graphene with various twist angles. We consider the advances in the emerging field of plasmonics in nanomaterials and give a comprehensive introduction to the basic theoretical models and techniques by using the linear response method.

* email: john.doe@physics.org

Strongly coupled fine particle clouds in fine particle plasmas

Hiroo Totsuji[1*]

[1]*Graduate School of Natural Science and Technology, Okayama University, Okayama 700-8530, Japan*

Fine particles of micron sizes in weakly ionized plasmas are usually negatively charged to large magnitudes and form classical strongly coupled plasmas. Lattice formations and other phenomena in their clouds have been investigated for more than 20 years under both gravity and microgravity. The basic nature of these clouds such as the characteristics of the electrostatic potential and their origin, however, are still mostly left unclarified. In this presentation, we point out that one of the most important effects of fine particles' existence is the large enhancement of the charge neutrality in their clouds which leads to the flatness of the potential/electric field[1-3]. Based on the drift-diffusion equations, particle simulations, and theoretical analysis[4], we show self-consistent structure formations of fine particles and compare the results with experiments in space and on the ground. An example of pysical quantities in the fine particle cloud under gravity is shown below.

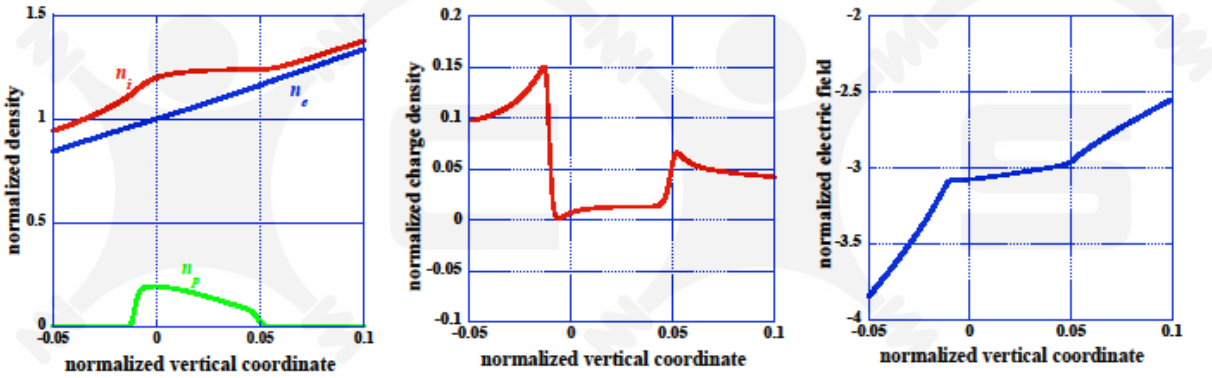

Figure: *Fine particle cloud under gravity; distribution of ions, electrons, and fine particles (left), net charge density (center) and electric field (right).*

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[*]*Professor Emeritus*
e-mail address: totsuji-09@t.okadai.jp

Strongly coupled dusty plasma in a 2D harmonic trap

Hong Pan[*1], Peter Hartmann[1, 2], Zoltan Donko[1, 2], Gabor J. Kalman[1], Marlene Rosenberg[3]

[1] *Department of Physics, Boston College, Chestnut Hill, Massachusetts, 02467, USA*
[2] *Institute for Solid State Physics, Wigner Research Centre for Physics, Hungarian Academy of Sciences, H-1525 Budapest, P.O. Box 49, Hungary*
[3] *Department of Electrical and Computer Engineering, University of California, San Diego, La Jolla, CA 92093-0407, USA*

All "2- dimensional" dusty plasma layers are in effect only quasi 2-dimensional [1], since they have a finite width, whose size is determined by the strength of the confining electrostatic trapping potential. The density profile and structure of such systems has been the subject of a number of recent works [2, 3, 4, 5, 6]. Most of these studies focused only on simulations. In this paper, we use the YOCP (Yukawa One-Component Plasma) model to describe the dusty plasma and provide a theoretical analysis based on the HNC approximation to obtain the density profile in a harmonic trap. Both of the cases of the plasma being in the liquid or solid phase are covered by the calculations. The formation of the density profile is controlled by the screening parameter κ, the coupling strength Γ and the trap strength. When Γ is high enough, the plasma always crystalizes, but the details of the liquid-solid phase boundary depend on all the parameters. As the trap strength is relaxed, the plasma splits into more and more layers. The number of layers is determined by the trap strength and kappa only, and for a given total layer width we can predict the number of layers. We also determine the phase boundary between the liquid and solid phases through the 2D pair correlation functions g(r) within the layers. These latter are provided by high quality MD simulations, which also provide density profiles for comparison with results obtained theoretically.

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*email: hongpb@bc.edu

Diffusion in two-dimensional quasi-magnetized rotating dusty plasmas

P. Hartmann[*1,2], **J. C. Reyes**[2], **L. S. Matthews**[2], **T. W. Hyde**[2], **R. U. Masheyeva**[3], **K. N. Dzhumagulova**[3], **T. S. Ramazanov**[3], **T. Ott**[4], **M. Bonitz**[4], **I. Korolov**[1], **Z. Donkó**[1]

[1] *Wigner Research Centre for Physics, Budapest, Hungary*
[2] *CASPER, Baylor University, Waco, Texas, USA*
[3] *IETP, Al Farabi Kazakh National University, Almaty, Kazakhstan*
[4] *ITPA, Christian-Albrechts-University, Kiel, Germany*

Transport phenomena in two dimensions are of ongoing interest due to unsolved theoretical challenges and the recent appearance of an increasing number of (effectively) two dimensional materials. Strongly coupled dusty plasmas have proven to provide unique possibilities for the microscopic understanding of classical macroscopic phenomena.

Transport properties of single layer dusty plasmas have been in the focus of strongly coupled dusty plasma research since the early years of the field. These efforts have provided very detailed analysis of the non-magnetized systems by means of both laboratory experiments and numerical simulations. Until recently, the effect that an external magnetic field played was accessible only through numerical investigations. This is due to the fact that experimentally, the application of real magnetic fields has shown to induce two fundamental problems, namely the disturbance of the background gas discharge and the need for unrealistically high magnetic fields to magnetize the dust component.

In our case the high quasi-magnetic field is experimentally applied to a single layer dusty plasma by rotating the particle cloud and observing the particle trajectories in a co-rotating frame. Based on the Larmor-theorem, effective magnetic fields up to 3000 Tesla can be achieved without disturbing the discharge. The self-diffusion in these quasi-magnetized strongly coupled systems is measured through the mean square displacement, and is compared to numerical simulations of magnetized two-dimensional Yukawa systems. Experiments and simulations show reasonable agreement supporting the predicted super-diffusion in such systems at the accessible time-scales.

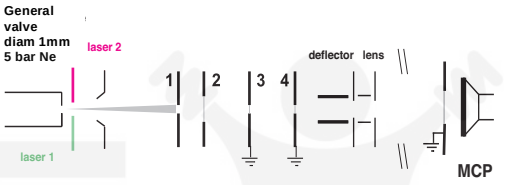
* email: hartmann.peter@wigner.mta.hu

Observation of a periodic many-body system

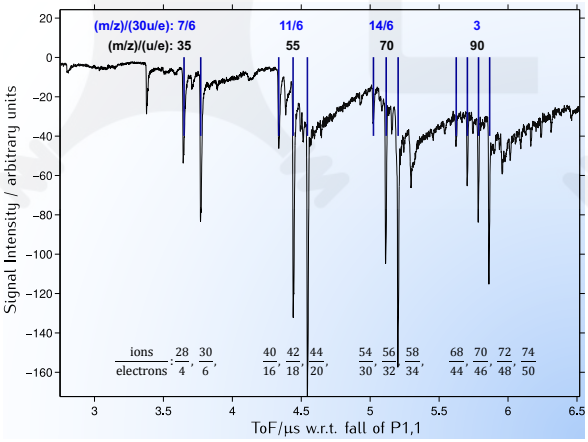
Klaus Müller-Dethlefs and François Michels

Photon Science Institute and School of Chemistry, Alan Turing Building
The University of Manchester, Manchester, M14 9PL, United Kingdom

We report the observation of a very surprising periodicity in a many-body system, in a long life-time (>0.3 ms) molecular Rydberg plasma. This is generated in the high-density high-collision rate region of a pulsed supersonic jet expansion by two-colour resonant excitation of nitric oxide (10%) in neon (5bar) into the high-*n* Rydberg threshold region close to the ionization limit. Considering the well-known properties of pulsed supersonic jet expansions and textbook plasma physics, plasma densities of $>10^{22}$ m^{-3} are reached in our experiments. For an initial electron temperature around 0.1K this suggests that the thermal electron *de Broglie* wavelength becomes larger than the mean electron separation and the electrons become *quantum degenerate* [1, 2].



The time-of-flight (ToF) mass spectrometer used is depicted in the figure above. Experimentally, two synchronous UV laser pulses produce the plasma a few mm away from the jet nozzle. After 170μs, when the plasma cloud is still *ca.* 130mm in front of aperture plate 1 (ap.1), two successive high-voltage (HV) pulses of 3.6 kV with a 0.2μs gap are applied to ap.1. The first HV pulse (P1,1; length 5.5μs) is followed by a gap of 0.2μs and a second pulse: P1,2. The observed ToF spectrum *w.r.t.* the falling slope of P1,1 is shown in the *lhs* figure (positive particle detection on MCP). The observed sharp peaks ("*slices*") in the ToF spectrum follow a fully reproducible progression of (*m*/*z*) mass to charge ratios (blue: *wrt* $m(NO^+)$=30u). From the *m*/*z* one obtains the corresponding ion to electron ratios of the 12 slices (bottom of figure).



In conclusion, we observe a many-body system consisting of a series of objects that contain a magic number of ions and electrons and that follow a periodicity. These objects are manipulated by fields in a ToF spectrometer without being destroyed, which shows that they behave as objects with a centre of mass.

email: k.muller-dethlefs@manchester.ac.uk

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Coupled electron-ion Monte-Carlo methods for warm dense hydrogen

Carlo Pierleoni[*1,2], D.M. Ceperley[3], M. Holzmann[4], and M.A. Morales[5]

[1]Department of Physical and Chemical Sciences, University of L'Aquila, Italy
[2]Maison de la Simulation, CEA-Saclay, France
[3]Department of Physics, University of Illinois at Urbana–Champaign, USA
[4]LPTMC, CNRS and University of Grenoble Alpes, Grenoble, France
[5]Physics Division, Lawrence Livermore National Laboratory, USA

The phase diagram of high pressure hydrogen is of great interest for fundamental research, planetary physics, and energy applications[1]. Laboratory experiments to reach the appropriate physical conditions are difficult and expensive, therefore ab-initio theory has played a crucial role in developing the field. The accuracy of the conventional method based on Density Functional Theory (DFT) is however limited and often non-predictive. We have developed a quantitative methodology based on Quantum Monte Carlo methods to study hydrogen in extreme conditions: the Coupled Electron-Ion Monte Carlo method (CEIMC)[2].

I will outline the main ingredients of the method and describe some applications to high pressure hydrogen. In particular I will focus on the the liquid-liquid phase transition, a first-order phase transition in the fluid phase between a molecular insulating fluid and a monoatomic metallic fluid. The existence and precise location of the transition line is relevant for planetary models. Recent experiments reported contrasting results about the location of the transition[3,4,5]. Theoretical results based on DTF are also very scattered [6,7,8,5]. We report accurate CEIMC calculations of this transition finding results that lie between the two experimental predictions, close to that measured in diamond anvil cell experiments but at 25-30 GPa higher pressure. The transition along an isotherm is signaled by a discontinuity in the specific volume, a sudden dissociation of the molecules, a jump in electrical conductivity and loss of electron localization[9].

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*carlo.pierleoni@aquila.infn.it

Ab initio Quantum Monte Carlo results for the Warm Dense Electron Gas

Tobias Dornheim[*1], Simon Groth[1], Travis Sjostrom[2], Fionn D. Malone[3], W.M.C. Foulkes[3], and Michael Bonitz[1]

[1] Institut für Theoretische Physik und Astrophysik, CAU Kiel, D-24098 Kiel, Germany
[2] Theoretical Division, Los Alamos National Laboratory, New Mexico 87545, USA
[3] Department of Physics, Imperial College, Exhibition Road, London SW7 2AZ, UK

The uniform electron gas (UEG) at finite temperature is of high interest for warm dense matter research, most notably as an input for thermal density functional theory. Until recently, the most accurate data had been obtained by Brown *et al.* [1] using quantum Monte Carlo (QMC) in the fixed node approximation (RPIMC) and by subsequently extrapolating the results for the finite model system to the thermodynamic limit by adding a finite-size correction. However, the quality of these results has been called into question: (I) RPIMC constitutes an uncontrolled approximation that induces errors of ~10% for the finite model system [2], and (II) the employed finite-size correction is only appropriate in parts of the warm dense regime. Here we show how to perform *ab initio* QMC simulations of the UEG without the fixed node approximation [3,4,5] and present a new extrapolation to the TDL without any systematic errors [6].
By carrying out extensive QMC simulations, we are able to construct an accurate (on the level of ~0.3%) parametrization of the exchange correlation free energy of the electron gas with respect to density, temperature, and spin-polarization covering the entire warm dense regime [7].

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* email: dornheim@theo-physik.uni-kiel.de

Nonequilibrium dynamics in the Hubbard model

Fabian Heidrich-Meisner[*1]
[1] *Arnold Sommerfeld Center for Theoretical Physics, LMU Munich, Germany*

The non-equilibrium dynamics of interacting fermions described by the Hubbard model and its relatives is attracting increasing attention, both because of the fundamental interest in the theoretically challenging regime and also because of significant experimental activities with strongly correlated electron materials and ultra-cold atomic gases in optical lattices.

The purpose of this talk is twofold. First I will give an overview over a range of non-equilibrium experiments carried our with ultra-cold quantum gases [1,2,3] to illustrate the capabilities of these systems. While initially, experiments focused on bosonic systems, the successful implementation of fermionic quantum gas microscopes in several groups will shift the focus to Fermi-Hubbard systems.

Second, I will introduce the time-dependent density matrix renormalization group (DMRG) technique, a numerical tool that provides accurate results at least on intermediate time scales for quasi-one dimensional systems. Applications of this technique to fermionic systems include interaction quenches [4], non-equilibrium mass transport [5], and the calculation of finite-temperature transport properties [6].
Finally, I will comment on prospects for investigating systems with long-range interactions with ultra-cold atomic gases and modifications of DMRG methods to deal with such systems.

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* email: heidrich-meisner@lmu.de

Quasi-adiabatic multi-shock compression of strongly coupled plasmas: correlations and degeneracy

V.E. Fortov*, R.I. Il'kaev, M.A. Mochalov, V.K. Gryznov, I.L. Iosilevskiy

Joint Institute for High Temperatures RAS, 125412, Izhorskaya st. 13, Bd.2, Moscow, Russia

A series of experiments with intense quasi-isentropic compression of plasma D2 and He were carried out to get strongly coupled plasma of deuterium and helium at an extremely high pressures and densities. Two-stage spherical explosively driven devices were used in these experiments. Accurate simultaneity of initiation of spherical high explosive charges provides a high symmetry of collapsing spherical steel shell which allows to achieve a high degree of spherical symmetry of the compressed plasma. Recordary high parameters of strongly coupled deuterium plasma were obtained through the experiments: pressures up to 11 TPa and density up to 10 g/cc. Helium plasma was compressed ~ 200 times up to density of 8 g/cc and pressures of P ~ 5 TPa. Multi-channel X-Ray complex registration consisting of three betatrons and a multi-channel optic-electronic system was used for registration of X-Ray images and diagnostics for the density of highly compressed plasmas of helium and deuterium. Pressure of compressed plasma was obtained by the hydrodynamic gas-dynamic calculations with the use of EOS taking into account non-ideality of the effects and real characteristics of all parts of experimental devices. Remarkable features of helium and deuterium plasma behaviour at these extremely high pressures, temperatures and densities are discussed with the use of simplified plasma models as well as of the results of computer simulation calculations using first principle approaches. The different theoretical models of plasma phase transitions in these conditions are discussed in comparison with shock wave experiments. Exclusively important role of quantum degeneracy effects as well as of strong correlation effects is analysed on the basis of the experimental data obtained.

* email: fortov@ficp.ac.ru

Brightness temperature and specific conductivity of multiple shocked initially gaseous protium and deuterium up to 0.4 TPa

D. N. Nikolaev[1], V. Ya. Ternovoi[1], A. A. Pyalling[1], A. V. Shutov[1]

[1] Institute of Problems of Chemical Physics of the Russian Academy of Sciences, Semenov str. 1, Chernogolovka, Moscow Region 142432, Russia

Brightness temperature records at wavelength of 600, 700, 734, 805, 807, 850, 900, 972 and 1500 nm from brass assemble with sapphire window, filled by gaseous isotope of hydrogen at initial temperature of 78 K and pressure of 25 or 9 MPa, was registered under its multiple shock compression up to 390 GPa. Electrical resistance of the compressed hydrogen layer was measured simultaneously by three electrode constant current measuring circuit. Process of compression was simulated by 1D and 2D hydrodynamic codes with use of wide-range semiempirical equation of state (EOS) of hydrogen and other assembly materials. Results of measurements were compared with simulation results, utilizing two hydrogen EOS models - SESAME and model with proposed metal - insulator transition. It was shown that hydrogen conductivity increases in small region of density in accordance with proposition of plasma phase transition existence in the investigated area of states of hydrogen, compressed by multiple shock.

High energy density plasmas diagnosed with X-ray free electron lasers

Ulf Zastrau[*1], K. Appel[1], C. Baehtz[2], S. Göde[1], Z. Konopková[1], M. Makita[1], M. Nakatsutsumi[1], A. Pelka[2], G. Priebe[1], A. Schmidt[1], K. Sukharnikov[1], T. Toncian, I. Thorpe[1], T. Cowan[2], T. Tschentscher[1]

[1] European XFEL, Schenefeld, Germany
[2] Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

The advent of the first free-electron X-ray lasers (XFELs), FLASH in 2004 and LCLS in 2009, may prove to be the most profound development since the invention of the laser and, equally, the synchrotron. Sharp improvements in a number of laser parameters, most notably intensity and pulse duration, support this expectation. This brings scientific dreams within reach. Indeed, the unprecedented opportunities and expectations have triggered considerable research activities worldwide. The talk will yield an overview of the experimental application of today's XFELs to explore matter in extreme conditions with advanced time-resolved x-ray methods.

In the near future, the High Energy Density Science (HED) instrument at the European X-ray Free-Electron Laser Facility in Hamburg, Germany, will allow investigations of an even wide range of materials and systems at extreme conditions. For sample excitation a variety of high energy drivers will be installed [1]. In particular, three separate optical laser systems will be available for warm- to hot-dense-matter creation, dynamic compression and laser-plasma interaction in electron-relativistic regime. These drivers will allow studying various phase space parameters with time-resolution down to 10 fs, pressures into the TPa regime, and electric field strength up to 10^{20} W/cm. This unique instrument is designed to enable the application of various x-ray probes including spectroscopic, diffraction and imaging methods [2]. It will operate in the photon energy range from 3 to 25 keV and will feature a variety of platforms facilitating the usage of different techniques in user-driven experiments. Future capabilities of the HED instrument, including the HIBEF user consortium contributions [3], will be presented along with selected science cases.

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* email: ulf.zastrau@xfel.eu

Exploring the physical properties of warm dense water by using Free-Electron-Laser

P. Sperling[*1,2], Z.Chen[1], C. B. Curry[3], M. French[4], J. B. Kim[1], J. Koralek[1], M. Mo[1], M. Nakatsutsumi[2], C. Rödel[5], S. Toleikis[6], P. Zalden[2], S. H. Glenzer[1]

[1] SLAC National Accelerator Laboratory, *Menlo Park, USA*

[2] *European XFEL GmbH, Hamburg, Germany*

[3] *University of Alberta, Edmonton, USA*

[4] *Universität Rostock, Rostock, Germany*

[5] *Friedrich Schiller Universität, Jena, Germany*

[6] *Deutsches Elektronen Synchrotron DESY, Hamburg, Germany*

Warm dense water is present in the interior of giant planets and its physical properties are critically important for modeling the interior structure of astrophysical objects and their temporal evolution. We present an experiment using a novel planar water jet operated in vacuum that is compatible with high repetition rate studies. The liquid density water is isochorically and uniformly heated to non-equilibrium warm dense matter by FLASH free-electron-laser irradiation (5.5 nm, 0.1-20 μJ). The ac conductivity can be extracted from optical transmission and reflection measurements on the picosecond timescale before significant expansion and subsequent relaxation occurs. Furthermore, the thermal electron-ion equilibration can be resolved from the temporal evolution of the optical transmissivity. The temporal evolution of the correlated water system is modeled by using radiation-hydrodynamic and DFT-MD simulations that allow comparisons with measured electrical conductivities and thermal electron-ion equilibration times.

*philipp.sperling@slac.stanford.edu

Viscosity, thermal conductivity and violation of the Wiedemann-Franz law in hydrodynamic electron liquids.

A. Principi*[1], M. Carrega[2], M. Polini[3], G. Vignale[4]

[1] Institute of Molecules and Materials, Radboud University, Nijmegen, The Netherlands
[2] CNR-NANO, Istituto Nanoscienze, Pisa, Italy
[3] Italian Institute of Technology, Genova, Italy
[4] University of Missouri, Columbia (MO), United States of America

Hydrodynamic flow occurs in an electron liquid when the mean free path for electron-electron collisions is the shortest length scale in the problem. In this regime, transport is described by the Navier-Stokes equation, which are controlled by three fundamental parameters, the bulk and shear viscosities and the thermal conductivity. In the hydrodynamic regime, the viscosities are entirely controlled by electron-electron interactions, while a strong violation of the Wiedemann-Franz law relating the thermal and charge conductivities is expected. I will present extensive results for the transport coefficients in the case of the two-dimensional massless Dirac fermion liquid in a doped graphene sheet, as well as recent experimental confirmations of our predictions.

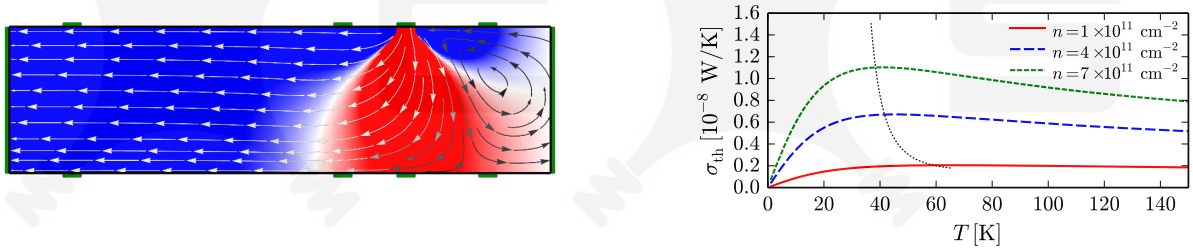

Figure: left panel: the electronic flow in graphene in the hydrodynamic regime (courtesy A. Tomadin). Right panel: the thermal conductivity of graphene stops following the Wiedemann-Franz law when it enters in the hydrodynamic regime.

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*a.principi@science.ru.nl

2D Plasma Condensation in Monolayer Semiconductors

Alexander Bataller[*1], **Kenan Gundogdu**[1]

[1] *Department of Physics, North Carolina State University, Raleigh, USA*

The physics of strongly coupled plasma finds validity in both real and quasiparticle charged systems. The temperature-density scaling relationships that determine many-body interactions, and ultimately condensation, is realized for the electronic excitation quasiparticle (exciton) in semiconductors. This relatively low-energy platform grants access to a parameter space occupied by liquid condensation and heavily influenced by quantum effects. In the nearly 50 years since its discovery [1], exciton condensation in semiconductors has been limited to cryogenic temperatures, and are often generated with high-intensity pulsed lasers [2,3]. Due to their quantum confinement, reduced material screening, and long charge lifetime, 2D semiconductors are ideal materials for high-temperature exciton condensation. We have recently discovered dense plasma condensation in 2D layered materials that can be created above room temperature using less excitation power than a laser pointer [4]. A description of this discovery and its implications will be presented.

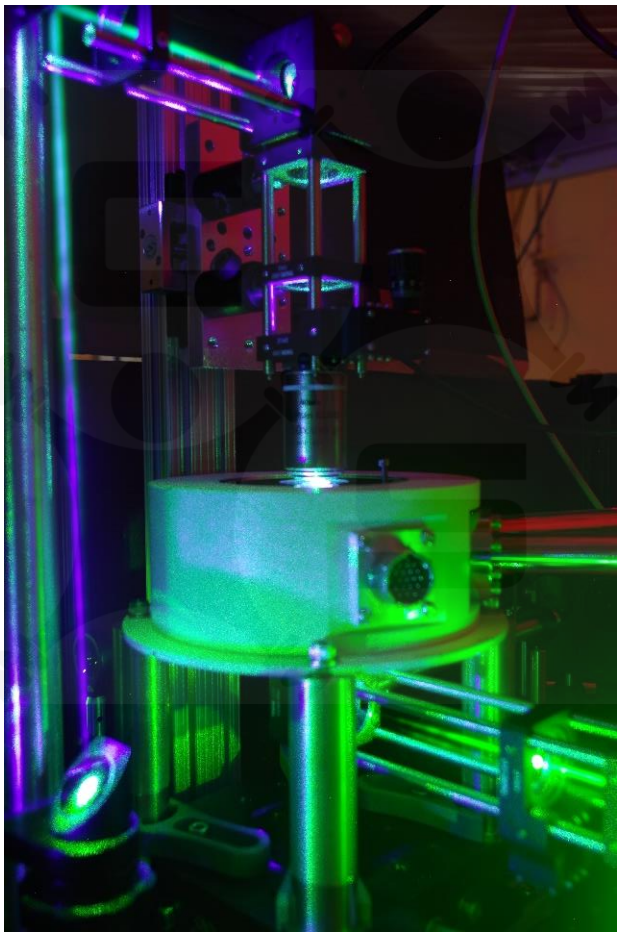

Figure: *Experimental photograph of laser-pumped plasma condensation in 2D semiconductors measured with photoluminescence microscopy [5].*

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* email: awbatall@ncsu.edu

Collective Behavior of Yukawa Systems

Luciano Silvestri[1], Gabor J. Kalman[1], Marlene Rosenberg[2], Zoltán Donkó[1,3], Peter Hartmann[1,3], Stamatios Kyrkos[4]

[1] *Department of Physics, Boston College, Chestnut Hill, Massachusetts, 02467, USA*
[2] *Department of Electrical and Computer Engineering, University of California San Diego, La Jolla, California, 92093, USA*
[3] *Institute for Solid State Physics, Wigner Research Centre for Physics, Hungarian Academy of Sciences, H-1525 Budapest, P.O. Box 49, Hungary*
[4] *Department of Chemistry & Physics, Le Moyne College, Syracuse, NY 13214, USA*

The Yukawa (or screened Coulomb) potential has been widely used as a theoretical model to describe a variety of many-body systems. Yukawa systems are completely characterized by the screening parameter, κ , and the nominal coupling strength, Γ . The detailed dynamics both of the single component (YOCP) and 2-component binary (Yukawa Binary Mixttures - YBM) are of great physical interest. Recent Molecular Dynamics (MD) computer simulations with improvements in the simulation technique have allowed us to obtain a large body of high quality data in the range Γ = {0.1 – 10,000} and κ = {0.5 -5} and have provided a wealth of new information on the dynamics of these systems. It is well known that the collective spectrum of the YOCP consists of a longitudinal acoustic mode, both in the weakly and strongly coupled regimes. In the long-wavelength limit the linear term in the dispersion (*i.e.* $\omega = sk$) defines the sound speed s . We present a detailed analysis of the evolution of the sound speed and damping of the oscillations from the weak through the strong coupling regimes, by examining the MD provided $S(k,\omega)$, the Dynamical Structure Function (DSF) data in the low frequency domain. We find that the damping at very low Γ values is basically a Landau damping, then at moderately weak coupling , $\Gamma < 1$, it is due to binary collisions; in the strongly coupled liquid regime quasi-localization seems to be the dominant mechanism.

This study is then extended to the YBM, whose weakly and strongly coupled spectra are less well-known. The theoretical analysis is pursued by using the Quasi Localized Charge Approximation (QLCA). It is predicted that at low coupling the collective spectrum is still characterized by a single longitudinal acoustic mode, while at higher coupling values the acoustic mode is accompanied by an optic mode, representing an out-of phase motion of the particles of the two species. It is also predicted that in the strong coupling regime, the oscillation frequency is governed by the heavier species, while in the weak coupling regime it is the lighter species that is dominant. Between the two extremes a coupling dependent effective mass prevails. The MD data, for the partial $S_{AB}(k,\omega)$ DSF-s, however, while in general, corroborate the QLCA results, reveal a much more complex picture, where the two modes are intertwined, and their behavior is highly dependent on the relative concentrations.

Structural and dynamic properties of strongly coupled dusty plasma of RF discharges

T.S. Ramazanov*[,1], N.Kh. Bastykova[1], A.U. Utegenov[1], A.Zh. Gabdulin[1], S.K. Kodanova[1], M.K. Dosbolayev[1], Z. Donko[2], P. Hartmann[2], and Zh.A. Moldabekov [1]

[1] *Institute of Experimental and Theoretical Physics, Al Farabi Kazakh National University, Almaty, Kazakhstan*

[2] *Institute for Solid State Physics and Optics, Wigner Research Centre for Physics, Hungarian Academy of Sciences, Budapest, Hungary*

Systems of charged dust particles in RF discharges attract huge interest due to the possibility of study of a variety of physical processes in the strongly coupled system of charged particles on a microscopic level. Following the intensive study of equilibrium or stationary non-equilibrium state of the system of dust particles [1], the interest has shifted to investigation of many-particle out-of-equilibrium systems. The methods of control of such system properties are intensively studied [1-3]. Simple and effective control in dusty plasmas is important for both theoretical study of strongly coupled out-of-equilibrium systems and their applications. In this article, the results of experimental and theoretical studies of the control over the system of dust particles by applying constant external field and using voltage waveform tailoring are presented [2-4]. Variations in the external field allow us to control the position of dust particles in the gas discharge and inter-dust particle interaction via changes in the gas discharge parameters and plasma polarization around the dust particle. The experiments clearly show changes in the structural properties of the system of dust particles with variation of the electric field at constant pressure and gas temperature. In order to understand the behavior of complex plasmas, the particle in cell simulation was used [2, 3]. Further, in order to study the possibility which this method offers for control of physical properties of the system of dust particles, the molecular dynamics simulations taking into account changes in plasma polarization around the dust particle were performed [5, 6]. It has been shown that this method makes it possible to manipulate both structural and dynamical properties of the system of dust particles effectively. This creates the basis for further experimental research of different processes in the charged strongly coupled out-of-equilibrium systems.

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* email: ramazan@physics.kz

Bow shock formation by supersonic flows in the presence of an obstacle in a two dimensional strongly coupled complex plasma

Harish Charan[1] and Rajaraman Ganesh

Institute for Plasma Research, Gandhinagar, Gujarat, INDIA

[1]Email: charan.harish@gmail.com

Supersonic flow past an obstacle is an ubiquitous phenomena in nature- for example in astrophysical systems, formation of bow shock structures created by solar winds in the magnetosphere of earth, fast moving comets, intersections of galaxies, to mention a few. Typically bow-shock-like structures are seen in these conditions.

Considering particles mediating via a Yukawa-type interaction as a prototype for a strongly coupled complex plasma, characterized by coupling strength (Γ, ratio of average potential to kinetic energy per particle) and screening parameter (k, ratio of mean inter-particle distance to shielding length), we address the fundamental problem of supersonic flow, U_0, past an stationary obstacle immersed in this strongly coupled system. We present the results on formation of bow shocks in complex plasma using first principle based classical molecular dynamics simulations. Depending on the values of Mach number $M_{CL} = U_0/C_L$, (where C_L is the longitudinal speed of sound), the bow shocks are found to be traveling or localized. The values of M_{CL} is taken in the range of $0.9 \leq M_{CL} \leq 4.4$. We find that for the transonic flows ($M_{CL} \lesssim 1.5$) the bow shocks travel in the opposite direction to the flow, for flows with $M_{CL} > 1.5$, the bow shocks are observed to be localized around the obstacle. The phase velocity of the traveling bow shocks are found to be independent of coupling parameter Γ, and decreases as the value of screen parameter is increased with functional dependency given by $\sim 1/k^{1.11}$. For flows with $M_{CL} < 2.6$, an emergence of secondary bow shocks behind the obstacle is seen, the secondary bow shocks are observed to travel in the downstream direction. To make possible connection with complex plasma experiments, the effect of neutral collisions on the bow shocks has been addressed, the details of which will be presented.

Corbino-disk and other viscometers for 2D quantum electron liquids

Andrea Tomadin[*1], **Giovanni Vignale**[2], **Marco Polini**[1]

[1] *Istituto Italiano di Tecnologia, Graphene Labs, Via Morego 30, I-16163 Genova, Italy*
[2] *Department of Physics and Astronomy, University of Missouri, Columbia, Missouri 65221, USA*

The shear viscosity is a fundamental property of many-body systems in the hydrodynamic regime which, in the case of quantum electron liquids, has been theoretically studied early on [1]. In Ref.[2] we proposed the first electronic viscometer, based on a Corbino-disk geometry (see figure). A strongly inhomogeneous tangential electric field produces a strain in the 2D quantum electron liquid on the disk surface. A dc electric potential difference between the inner and outer rim of the Corbino disk arises, from which the value of the viscosity can be determined.

Successive experimental [3] and theoretical [4,5] works considered simpler geometries in graphene Hall bars or half-planes [6], where a dc current is sufficient to exert a strain on the electron liquid and the non-local resistance measured between neighboring contacts allows to determine the value of the viscosity.

A.T. and M.P. are supported by the European Union's Horizon 2020 research and innovation programme under grant agreement No. 696656 "Graphene Core1".

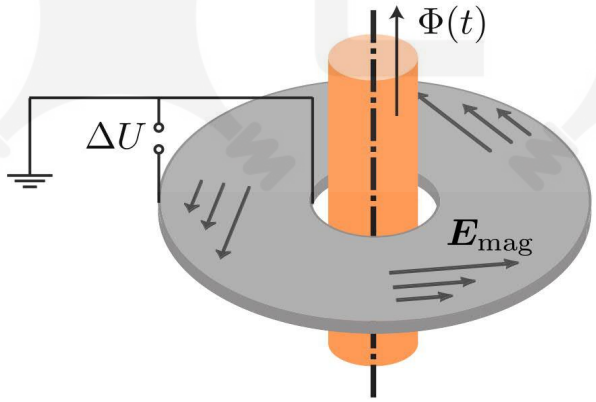

Figure: *A dc electric potential difference ΔU is generated by an ac magnetic field Φ(t) threading the inner hole of a Corbino disk setup. The magnitude of the potential and its dependence on the frequency of the magnetic field allows to determine the viscosity of the 2D quantum electron liquid on the disk surface. The viscous response is elicited by the stress exerted by the induced tangential electric field E_{mag}, which decreases along the radius of the disk.*

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* email: andrea.tomadin@iit.it

Plasmon properties in dilute, two-dimensional electron liquids

Dominik Kreil*, **Clemens Staudinger, Katharina Astleithner, Helga M. Böhm**

Institut für Theoretische Physik, Johannes Kepler University, 4040 Linz, Austria

Two-dimensional (2D) electron systems, where presently Dirac liquids and insulating oxide surfaces deserve much attention, have remained a topic of significant importance also in semiconductor heterostructures. Compared to bulk systems, the 2D realizations show much more pronounced correlations, key examples being the collective modes such as plasmons and magnons. For highly dilute semiconductor quantum wells [1] it is mandatory to account for dynamic multi-particle fluctuations, in particular two-particles-two-holes (2p2h) excitations [2]. This dynamic pair theory yields a substantially lower plasmon energy than static theories [3, 4], and, consequently, a much smaller critical wave vector for Landau damping (Fig. 1). The plasmon broadening by pair excitations turns out to be rather small. The next step is the extension to spin-sensitive effective interactions to study the spin-spin and the spin-density linear response functions. These promise new insights via the longitudinal spin plasmon and a highly interesting 'magnetic antiresonance' [4]. We discuss unfamiliar excitation regimes in the partially spin-polarized electron liquid where one (the spin-density response) or both (spin-spin response and spin-density response) vanish.

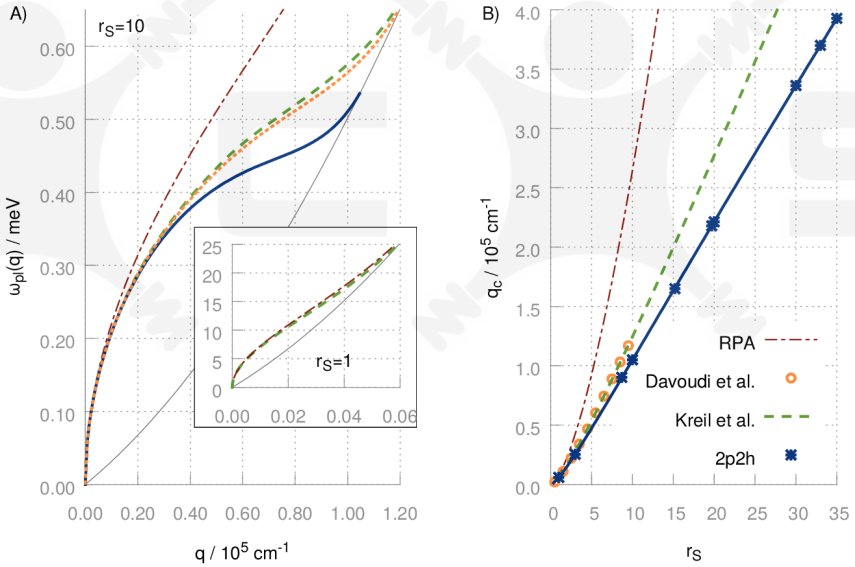

Figure 1: Plasmon disperson (left) and critical wave vector (right) in the random phase approximation (RPA, red, dashed-dotted) lines, for two static generalized RPA approaches (Ref. [1], yellow dots, and Ref. [4], green, dashed lines), and in the dynamic 2-pair theory (blue, solid lines). The density parameter r_s = 10 corresponds to the GaAs-AlGaAs quantum well of Ref. [1] with an areal density of 2 10^{13}/cm^2.

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* email: dominik.kreil@jku.at

Graphene Plasmonics

Ben Van Duppen*

Department of Physics, University of Antwerp, Belgium

With the advent of graphene, a two-dimensional carbon allotrope, about ten years ago [1], a completely new branch of condensed matter physics was born. This branch turned out to be exceptionally interdisciplinary with connections to many different subfields of physics, chemistry and engineering [3]. Since then, many other two-dimensional crystals were synthesized resulting in a completely new class of two-dimensional materials featuring many unconventional properties.

As graphene hosts a two-dimensional liquid of charge carriers, albeit behaving as massless Fermions, it is electronically conductive and capable of supporting collective oscillations, better known as plasmons. In this way, the field of graphene physics and plasmonics were merged [3] and it was shown that plasmons in graphene can exist with exceptional properties.

In this talk, I will briefly give an overview of the field of graphene plasmonics, the challenges faced along the way and where we stand today. I will end with giving two examples of how graphene plasmonics can be used to probe many-body properties of the electron liquid [4s] and how it can make graphene a strongly nonlinear optical material [5].

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* email: ben.vanduppen@uantwerpen.be

Superionic phases in C-N-O-H mixtures and the interior of Neptune-like planets

Martin French[1]

[1]*University of Rostock, Rostock, Germany*

The nature of molecular substances like water, ammonia, and methane changes drastically upon strong compression to the Mbar regime. Computer simulations based on density functional theory predict that water and ammonia dissociate fully into charged particles. Depending on the temperature, this results in the formation of phases of ionic ices, conducting liquids, or superionic solids [1]. The latter are characterized by mobile protons diffusing through a solid oxygen or nitrogen lattice. In contrast, methane decomposes into long-chained hydrocarbons or diamond [2].
This talk will give an overview of the predicted high-pressure phase diagrams of water, ammonia, methane, and their mixtures with emphasis on the superionic phases. Fundamental properties like the equation of state and the electrical conductivity will be discussed [3,4]. The relation to current experimental approaches to measure superionicity at high pressures will also be given.
Our solar giant planets Uranus and Neptune are rich in warm dense mixtures of water, ammonia, and methane. Thermodynamic states in their deep interior correspond well to conditions at which superionic phases are predicted. The possible occurrence of superionic water-ammonia phases alongside methane decomposition provides an immense amount of possibilities for layer formation and compositional differentiation. Therefore, understanding the physical behavior of warm dense C-N-O-H mixtures is key to explaining yet unsolved puzzles regarding Uranus' and Neptune's strong difference in luminosity or the generation of their complex magnetic fields [5,6].

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Electrical Conductivity for Warm Dense Matter

James Dufty[*1], **Kai Luo**[1,2], **S.B. Trickey**[1,2]

[1] *Department of Physics, University of Florida, Gainesville, FL, USA*
[2] *Quantum Theory Project,University of Florida, Gainesville, FL,USA*

Current studies of transport properties for conditions of warm dense matter typically combine a mean-field DFT dynamics for electrons while treating the ions as a static disordered background [1]. The ion average is implemented by AIMD with the electronic transport coefficient calculated at selected time steps (snapshots). Alternative calculations based on electron quantum kinetic theory also assume this model of ions providing a disordered background for the dynamic electrons [2]. Two questions arise: what is the origin of the mean field approximation in the first case, and how should these analyses be extended to include the self-consistent treatment of ion dynamics? Here we address the latter problem in the context of the mean-field approximation for the electron Hamiltonian. Attention is restricted to the electron conductivity for simplicity. Starting from the Green-Kubo expression, the current-current autocorrelation function is described as an electron-averaged time correlation function whose dynamics is parametrized by a history (trajectory) of the ions, followed by an average over ion histories. In the limit of immobile ions, this result reduces to the currently used Kubo-Greenwood conductivity [1] for a given fixed ion configuration, with subsequent average over configurations. More generally, the dynamics of the electrons and ions are intimately coupled. However, due to the simplifications of the mean-field approximation the result can be expressed in terms of Kohn-Sham eigenvalues and orbitals calculated at each time step of an AIMD simulation for the ions. The importance of ion dynamics for the conductivity calculation is illustrated with a simple example, based on modification of a recently developed Kubo-Greenwood package [3].

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* email: dufty@phys.ufl.edu

Oscillating ions: from strong coupling to fusion temperatures

Yu. K. Kurilenkov[1], V.P.Tarakanov[1] and S.Yu.Guskov[1,2]

[1]Joint Institute for High Temperatures, RAS, Moscow, Russia

[2]Lebedev Physical Institute, RAS, Moscow, Russia

Inertial electrostatic confinement (IEC) fusion represents rather old branch of controlled thermonuclear synthesis study [1-3]. However, at traditional schemes of IEC the high fusion power density is incompatible with high efficiency $Q = E_{fusion}/ E_{input}$, since "beam"-like distribution of ions by energies is smoothed essentially by Coulomb collisions before the synthesis is realizing. To overcome this problem, at the end of 90-th it have been suggested at LANL [4] to inject the electron beams into internal space of grid-like cathode sphere. In this case the potential (like parabolic one) will appear at interelectrode space, where the ions will undergo harmonic oscillations. This variant of IEC have been titled as periodically oscillating plasma spheres (POPS), and this scheme have been demonstrated at experiment successfully also [5]. At the moment of throw out the ions are practically stopped, and ions subsystem turns out to be strongly coupled. At the next moment the potential well of virtual cathode (VC) do accelerate ions up to fusion energies at the "bottom", where head-on collisions, for example, of deuterons leads to DD synthesis with corresponding neutron yields. Periodic collapses of ions provide the pulsating neutron yield. At the present work the results of PIC modeling of particle dynamics and neutrons yield are compared with the experiment, where IEC with POPS-like scheme with VC have been realized on the basis of nanosecond vacuum discharge (NVD) in cylindrical geometry [6]. At this case we don't need to inject synchronized electron beams additionally (as in [5]) since we have the streams of autoelectrons from cathode which are appearing automatically when the voltage applied. The results of PIC modeling of proton– boron nuclear burning ($p+ {}^{11}B \rightarrow \alpha + {}^{8}Be \rightarrow 3\alpha$) at IEC scheme based on NVD are presented and discussed also [7].

This work was supported by a grant No. 14-50-00124 of the Russian Science Foundation.

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email: kurilenkovyuri@gmail.com

Direct determination of dynamic properties of strongly coupled plasmas

I.M. Tkachenko*[1], Yu.V. Arkhipov[2], A.B. Ashikbayeva[2], A. Askaruly[2], L. Conde[3], A.E. Davletov[2], Z. Donkó[4], D.Yu. Dubovtsev[2], P. Hartmann[4], I. Korolov[4], S. Syzganbayeva[2]

[1] Universidad Politécnica de Valencia, Valencia, Spain
[2] Al-Farabi Kazakh National University, Almaty, Kazakhstan
[3] Universidad Politécnica de Madrid, Madrid, Spain
[4] Wigner Research Centre for Physics, Budapest, Hungary

A closed algorithm is suggested which allows the determination of dynamic characteristics of various strongly coupled plasmas (one- and two-component plasmas, electron gas, etc.) within the non-perturbative model-free moment approach without any data input from simulations or direct experiments. The standard Nevanlinna formula (see [1,2] and references therein) for the loss function (LF) which incorporates its independently calculated power frequency moments or the sum rules is complemented with an observation with respect to the LF low-frequency behavior [2]. Thus, the constructed LF satisfies all involved sum rules automatically and permits to determine the system's dynamic structure factor (DSF), the dispersion, the decay, and other characteristics of the collective modes using only the (partial) static structure factors obtained numerically or theoretically. For one-component plasmas it also provides a model for the dynamic local-field correction [3]. Simplified interpolation formulas for the LF moments, which do not need the external static data, are also suggested whose validity confirms the robustness of the present approach. A good quantitative agreement with molecular dynamics simulation data is achieved in a wide realm of variation of the system parameters, see, for example, the following figures where our results computed on the basis of static characteristics obtained by the molecular-dynamics (MD) method are compared to the MD dynamic data.

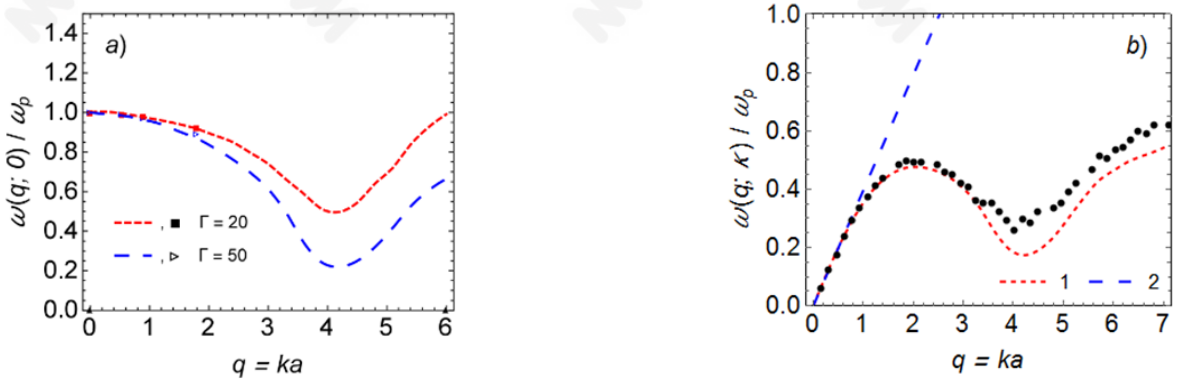

Figure: *Dispersion of plasma modes compared to MD data (figures): a) Coulomb OCP, b) Yukawa OCP at Γ=100 and κ=2. Line 2 stands for the sound mode. a is the Wigner-Seitz radius.*

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* email: imtk@mat.upv.es

Enhancement of nuclear fusion reactions in asymmetric binary ionic mixtures

J. Clérouin *[1], **Ph. Arnault**[1], **N. Desbiens**[1], **A. White**[2], **C. Ticknor**[2], **J. D. Kress**[2], and **L. A. Collins**[2]

1 *CEA, DAM, DIF, 91297 Arpajon, France.*
2 *Theoretical Division, Los Alamos National Laboratory, NM 87545, USA.*

Using orbital free molecular dynamics simulations (OFMD) [1], we studied the properties of asymmetric mixtures such as hydrogen-carbon, hydrogen-aluminum, hydrogen-copper [2], and hydrogen-silver [3]. By comparing the pair distribution functions (PDF), we found that the structure of the heavy component closely resembles an effective one component plasma (OCP) [4] unlike its light counterpart. This effect results from the diminution of the effective accessible volume triggered by the highly-charged components. This over-correlation translates into a strong enhancement of nuclear reactions, which is evidenced by the calculation of the H factor using the Widom expansion.

* jean.clerouin@cea.fr

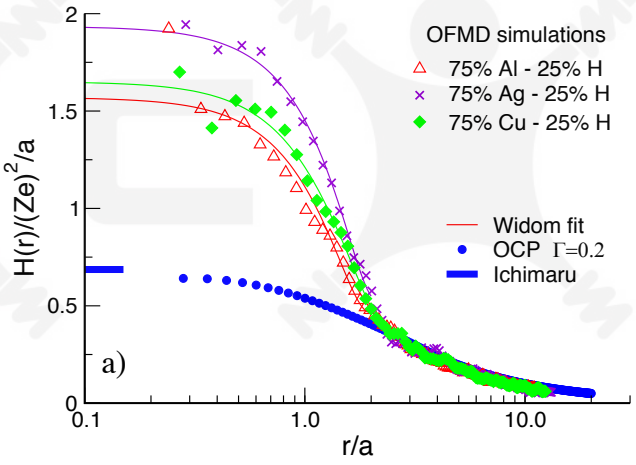

Figure: *Nuclear reaction enhancement factor for hydrogen H(r) for a H-Z mixture (Z=Ag, Cu, Al) at 75% heavy concentration computed with OFMD simulations. The thin line is the short distance Widom expansion of the PDF. The blue curve gives the corresponding one component plasma result that does not account for mixture effects.*

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Statistical properties of microfields in multicomponent coupled plasmas

S. Ferri*[1], A. Calisti[1], C. Mossé[1], B. Talin[1]

[1] Aix-Marseille Université, CNRS, PIIM UMR 7345, F-13397 Marseille, France

The radiative properties of an emitter surrounded by a plasma are modified through various mechanisms. One of the most important mechanism in hot and dense plasmas, is the broadening of emitted line shape of bound-bound transitions, due to coupling of the dipole moment with the local electric field produced by the plasma electrons and ions. Characterizing properly those electric microfields is very important for spectroscopic diagnostics as their statistical properties are principal ingredients of line shape standard theories.

A classical molecular dynamics code, the BinGo-TCP code [1], has been developed to simulate neutral multi-component (various charge state ions and electrons) plasmas. This technique involves the mechanism of collisional ionization recombination necessary to simulate plasmas with a definite temperature and equilibrated populations of ions of various charge states. As the particle environment is explicitly described, this method gives access to different quantities of interest (positions, velocities, ionic charges, energies) and their statistical static and dynamics properties (pair correlation functions, ionization potential depression, etc.), [2,3].

Among other properties, we report here investigation on statistical properties of microfields in multicomponent coupled plasma composed of various ionic charges and electrons. Via the analysis of the field histories at the effective charges, the field distribution or correlation functions can be inferred to study the influence of the correlations between ions or electrons or both, [4].

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Periodic states in the homogeneous two dimensional electron gas at all densities.

Bernard Bernu*[1], François Delyon[1], Markus Holzmann[2]

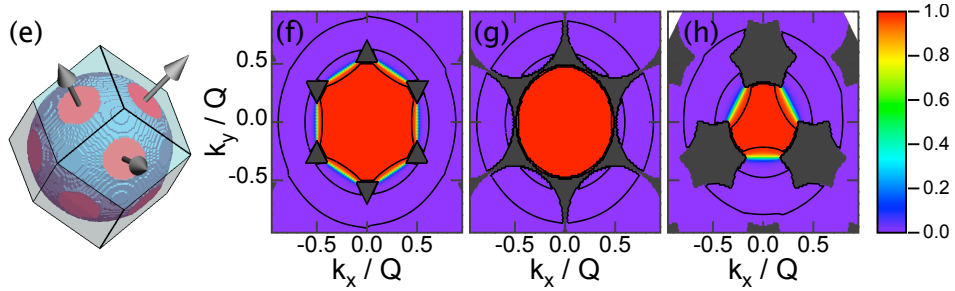
[1] *LPTMC, CNRS / University P&M Curie, Paris, France*

[2] *LPMMC, CNRS / University Grenoble Alpes, Grenoble, France*

The simplest electronic model is the jellium, i.e. an homogeneous electron gas embedded in a back-ground of opposite charge such that the system is neutral. This model is a good start to study alkali metals such as solid sodium. At zero temperature, the only parameter of this model is the density. Electrons interact through the Coulomb potential $1/r$. At low densities, the potential energy decreases less slowly than the kinetic energy and this is the classical limit. At zero temperature, electrons make a crystal called the Wigner crystal. In the opposite limit of high densities, the kinetic energy dominates and form ultimately a quantum Fermi gas. Understanding the intermediate regime is a challenging task.

The mean field solution of the jellium is called the Hartree-Fock approximation (HF). Within HF, Overhauser(1962) has shown that the Fermi gas is unstable under a spin density wave (SDW). In spite of this theoretical prediction, until very recently, the ground state phase diagram of the jellium was known as various Wigner crystals at low density and the Fermi gas at high density with a transition at $r_s \approx 4$.

We present solutions which interpolate between the Wigner crystal and the Fermi gas, first within Hartree-Fock (HF) approximation (see for example the Figure representing n(k) for BCC lattice symmetry) and then on going work using Quantum Monte Carlo. At high densities the HF solutions look like the SDW proposed by Overhauser. We have improved his method and evaluated quantitatively the high density limit.



* email: bernu@lptmc.jussieu.fr

Non-linear Screening Effect on Parameters of Phase Transitions and Boundaries of Complex Plasma Thermodynamic Stability (on the Phase Diagram)

Martynova I.A.[*1,2], **Iosilevskiy I.L.**[1,2], **Shagayda A.A.**[3]

[1] *Joint Institute for High Temperatures RAS, Moscow, Izorskaya 13 Bldg2, Russia, 125412*
[2] *Moscow Institute of Physics and Technology (State University), Dolgoprudny, Institutskiy Lane 9, Moscow region, Russia, 141700*
[3] *State Scientific Center of the Russian Federation Federal State Unitary Enterprise Keldysh Research Center, Moscow, Onezhskaya 8, Russia, 125438*

Applicability limit of the well-known phase diagram [1] for complex (dusty, colloid, etc.) plasma are under discussion. Existence of finite density gap at all phase boundaries at this diagram was claimed earlier [2]. Existence of extensive domains with violation of thermodynamic stability conditions (i.e. with negative isothermal compressibility $\left(\partial P/\partial \rho\right)_T<0$ was also claimed [2] if one uses well-known non-ideal equation of state corrections by Hamaguchi et al.[1], S. Khrapak et al.[3], etc. Present work is devoted to analysis of a range of applicability for basic assumption in Hamaguchi's phase diagram [1] i.e. linearized (Debye) screening of macroions by microions, which leads to the Yukawa form for effective interactions between macroions. Parameters of *non-linear screening* for macroions were calculated within direct Poisson-Boltzmann approximation. Two basic effects were revealed as a result of such calculations: (*i*) – decomposition of all microions onto two subclasses, free and bound ones, and (*ii*) – significant reduction of "visible" (effective [4]) charge Z^* of initial bare macroion Z under non-linear screening by small high-density envelope of bound ions. This *renormalization* of initial Z and macroion concentracion at the border of the cell (or at infinity if there is no cell concidered) n into Z^* and n^* ($Z^* < Z$ and $n^* < \dot{o}n$) leads to corresponding renormalization of initial Γ and κ into Γ* and κ^* (Γ* < Γ and $\kappa^* < \kappa$). The main physical assumption of the present work is that phase state (e.g. solid, fluid etc) of complex plasma under non-linear screening is still the same as in the initial Hamaguchi's diagram, but in κ^*–Γ* plane instead of κ–Γ one. Corresponding calculated shifts of phase boundaries in the initial Hamaguchi's diagram, i.e. triple point, melting and bcc-fcc boundaries, are discussed and illustrated. The work is supported by the Russian Science Foundation (grant No. 14-50-00124).

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* email:martina1204@yandex.ru

Enthalpic and entropic phase transitions in strongly coupled plasmas

Igor Iosilevskiy*

Joint Institute for High Temperature (Russian Academy of Science)
Moscow Institute of Physics and Technology (State University)

Remarkable features of entropic 1st-order phase transitions (*S*-PT) [1,2] are under discussions in comparison with ordinary well-known enthalpic (VdW-like) phase transitions (*H*-PT). The basic “driving” mechanism for many *S*-PT is *forced decomposition* of bound complexes – atoms, molecules, clusters etc. [3,4] up to the forced deconfinement of hadrons to constituent quarks in interiors of neutron stars [5,6]. The key feature of *S*-PT is negative sign of its latent heat and consequent falling *P*(*T*) dependence for phase coexistence line. Thermodynamics of *S*-PT is much more complicated than that of *H*-PT. In particular, isostructural *S*-PT is always internal part of more general thermodynamic anomaly – extended domain with anomalous (*negative*) sign for wide set of (usually positive) second cross derivatives of thermodynamic potential, e.g. Gruneizen coefficient, thermal expansion coefficient, (isochoric) thermal pressure coefficient etc. Negative sign of all the derivatives leads to violation of standard behavior and relative order for many iso-lines in *P*–*V* plane, e.g. isotherms, isentropes, shock adiabats etc. Entropic PTs (e.g. ionization- and dissociation-driven PTs) have more complicated topology of stable and metastable domains in their two-phase region in comparison with ordinary (i.e. VdW-like) enthalpic PTs. Anomalous thermodynamic features of entropic PTs have simple geometrical interpretation – multi-layered structure of thermodynamic surfaces for temperature, entropy and internal energy as a pressure-density functions, e.g. for *T(P,V), S(P,V)* and *U(P,V)*. Discussed anomalies are illustrated for examples of entropic phase transitions revealed experimentally as well as by calculations via simplified plasma models and via first-principal approaches for dissociation- and ionization-driven phase transitions in WDM of hydrogen, nitrogen and other strongly coupled materials.

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* email: ilios@ihed.ras.ru

Screened cluster equation of state for the hydrogen-helium mixture

Vincent Ballenegger[*1], **David Wendland**[1,2], **Angel Alastuey**[2]

[1] *Institut UTINAM, Univ. Bourgogne-Franche-Comté, UMR CNRS 6213, Besançon, France*
[2] *Laboratoire de physique, École Normale Supérieure de Lyon, UMR CNRS 5672, Lyon, France*

The description of a hydrogen-helium gas within the physical picture, that is in terms of Coulomb interactions between the constituent quantum point particles (electrons, protons and helium nuclei), is well suited for deriving highly accurate equations of state in various regimes, as needed for instance in stellar modeling. Using the equivalence with a classical gas of loops provided by the path integral approach [1], the fugacity expansion of the grand-potential, or of any other equilibrium quantity, can be expressed in terms of Mayer diagrams. These diagrams are non-perturbative with respect to the Coulomb interaction and thus account for effects involving arbitary high orders in the charges. The Coulomb divergencies are eliminated by performing systematic chain resummations, leading to a new Mayer-like diagrammatical series [1,2] where the loops interact via an integrable effective potential which is closely related to the RPA interaction.

Starting from the fugacity series for the grand-potential, we performed both path integral Monte Carlo computations and analytical calculations to evaluate all Mayer-like diagrams which describe at most 3 particles interacting via the effective potential. The resulting particle densities are inferred *via* the usual thermodynamical relation, while charge neutrality is easily enforced by a straightforward diagrammatical prescription. After eliminating the fugacities in favor of the densities, we obtain the Screened Cluster equation of state at 3rd order (SC3 EOS) [3,4]. Interestingly, that equation may describe regimes where arbitrary fractions of the elementary constituents are recombined into ions or atoms.

The SC3 EOS accounts for modifications of the vacuum virial functions with increasing density due to shifts as well as broadening of spectral lines. Three-body effects like the formation of helium atoms or atom-charge interactions are computed without recourse to an intermediate modelization or *ad-hoc* prescriptions for bound states contributions. The predictions of the semi-analytical SC3 EOS are eventually compared with those of the tabulated OPAL equation of state.

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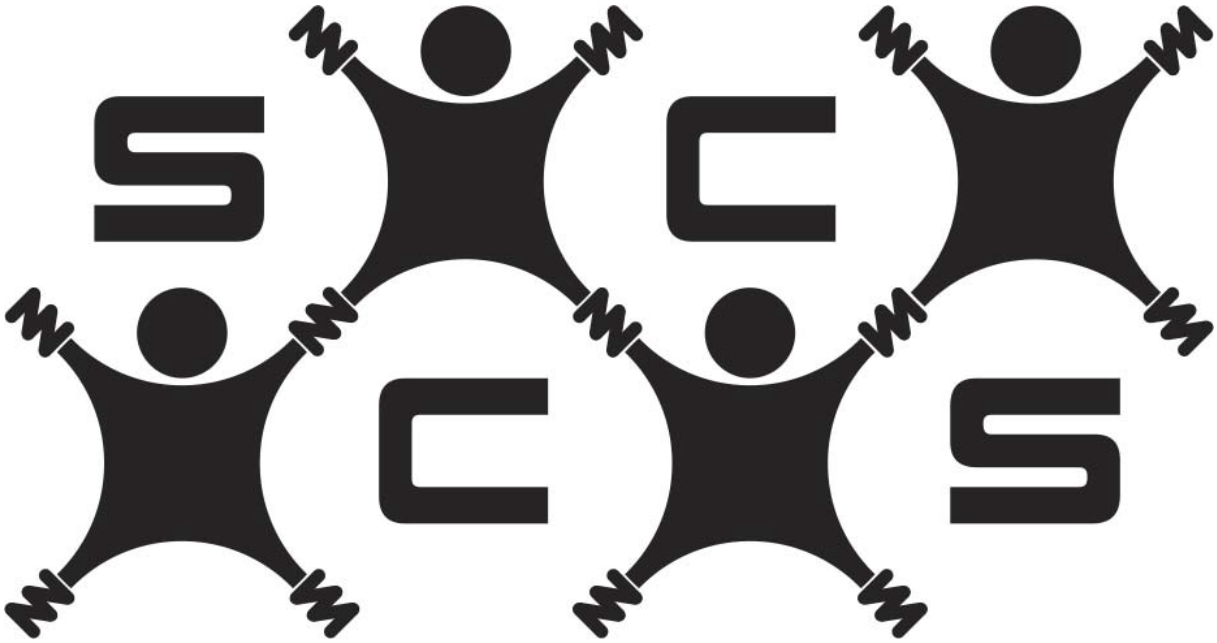
* email: vincent.ballenegger@univ-fcomte.fr

Poster Presentations



An equation of state for $CaCO_3$ at high pressures and temperatures

A.A. Rykounov

Russian Federal Nuclear Center – All-Russian Research Institute of Technical Physics (RFNC-VNIITF), 456770, Vasiliev street 13, PO box 245, Snezhinsk, Chelyabinsk region, Russia

From the standpoint of polymorphic transformations, calcium carbonate is a rather complicated compound: the number of its phases which were observed experimentally or predicted theoretically approaches ten. What adds more complexity is the fact that calcite-I – a thermodynamically stable state of $CaCO_3$ under ambient conditions – tends to form metastable modifications. That is why it is a problem to determine phase stability boundaries for $CaCO_3$, and discussion in the scientific literature continues up to now.

In this work we examine stability boundaries for three stable phases (calcite-I, aragonite and post-aragonite) and two metastable phases (calcite-III and calcite-VI) of $CaCO_3$ using the pseudo-potentials approach within density functional theory. It is shown that the state-of-the-art functionals PBESol and AM05 predict the equilibrium cell parameters of the phases, cold compression curves, and some mechanical properties better than the traditionally used PBE and LDA.

Quantum molecular dynamics is used to derive an equation of state (EOS) for $CaCO_3$ at temperatures 300 – 63000 K and densities 1.585 – 7.943 g/cm^3. For model systems, super-cells of calcite-I and aragonite are used, as well as a cubic super-cell containing 25 molecules of $CaCO_3$ that helped obtain thermodynamic parameters for liquid and amorphized calcium carbonate. The Hugoniot curve obtained from the EOS (the highest pressure 1.17 TPa at density 7.54 g/cm^3) agrees well with data from shock experiments reported in [1] and [2].

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arykounov@gmail.com

Plasma polarization in compact stars

Igor Iosilevskiy*

Joint Institute for High Temperature (Russian Academy of Science)
Moscow Institute of Physics and Technology (State University)

Macroscopic plasma polarization, which is created by gravitation and other mass-acting forces in massive astrophysical objects (MAO), is under discussion. New “non-ideality force” due to effects of strong Coulomb interaction of charged particles was claimed [1] as significant additional source of such polarization. Standard description in local (LDA) approximation is well-known (e.g. [2]). Simplified situation of totally equilibrium isothermal compact star without magnetic field and relativistic effects is considered in present work. The study based on multi-component version of variational formulation of equilibrium statistical mechanics. Compact and general (non-local) formula is presented as general solution of the problem [3]. It includes naturally all non-ideality effects within main Jakoby matrix for densities on chemical potentials. One of the significant consequences of this formula is prediction of possibility for macroscopic charge localization [4] at any phase interface or at any other discontinuities in homogeneous thermodynamic profiles in interiors of compact stars.

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* email: ilios@ihed.ras.ru

Effect of electron collisional and radiative broadening of super-transition arrays on plasma opacities

A.A. Ovechkin*, **P.A. Loboda**

Russian Federal Nuclear Center – All-Russian Scientific Research Institute of Technical Physics, Snezhinsk, Chelyabinsk Region, Russia

Monochromatic and mean plasma opacities may strongly depend on electron collisional and radiative spectral-line broadening in certain plasma temperature and density domains. We propose a method to allow for the relevant broadening mechanisms in the framework of the superconfiguration approach [1]. In so doing, electron-configuration decay rates are averaged by using suitable weighting factors being specific for one-electron transition of interest and providing proper absorption cross-sections at the wings of the spectral-line arrays. Electron-configuration decay rates are expressed through the one-electron radiative and electron-collisional excitation/deexcitation rates calculated by the RESEOS code [2] with average-atom electron wave functions. The one-electron collisional excitation/deexcitation rates are calculated in the plane-wave Born approximation.

RESEOS opacities obtained with the account of electron collisional and radiative broadening of super-transition arrays are compared with the results of more detailed Opacity Project [3] and ATOMIC [4] calculations. Generally, the widths of spectral-line arrays obtained with RESEOS are greater than those ones given by the ATOMIC model but agree well with the Opacity-Project data.

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* email: ovechkin.an@mail.ru

DENSE PLASMA AS A NON-LINEAR MATTER

George A. Pavlov*
Institute of Problems of Chemical Physics RAS, 142432 Chernogolovka, Moscow Region, Russian Federation, e-mail: pavl4411@yandex.ru

Theoretical investigations of thermodynamic, transport (rheology), and optical characteristics of non-ideal media, which are characterized by a strong interaction between particles, are based on linear and non-linear response theory.

A variant of non-linear response theory [1] is offered to describe the nonlinear interaction of electric and electromagnetic waves in a charged dense matter: plasma echo, waves transformations, second harmonic generation, and nonlinear interaction of charged particles with non-ideal charged matter (nonlinear stopping power). A new model approach described these phenomena is the following. It is possible to consider the correct forms of nonlinear response functions and time correlation functions as explicit approximations with several fitting parameters. The definition of the parameters is carried out from known frequency moments of nonlinear response functions (or time correlation functions) and other exact relations (sum rules) for these functions. For the first time some characteristics of mentioned above nonlinear phenomena, allowing comparison with experiments, have been determined for dense charged media.

The non-linear kinetic (transport) coefficients for a non-ideal multicomponent charged medium (plasma) were defined according to the version of the theory of non-linear response to thermal perturbations [2]. The approach [2] is based on comparison of phenomenological conservation equations for a charged continuous medium and equations of motion for the operators of the corresponding dynamic variables in the form of generalized Langevin equations. The formal definitions of the non-linear and linearized (Burnett) kinetic coefficients in terms of long-wave and low-frequency limits of the corresponding correlation functions of non-ideal charged and neutral mediums are presented in compact form. These results can be used for continuous charged media: one and two component Coulomb systems, electrolytes, liquid metals, and nuclear matter, as well as for dense neutral media. First calculation is carried out of the linearized Burnett kinetic coefficients for model two-component Coulomb systems. The use is briefly discussed of Burnett kinetic coefficients to emphasize that knowledge of the values of such coefficients needed to solve a number of high-temperature hydro-and gas dynamics problems for dense media [3].

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*) *e-mail: pavl4411@yandex.ru*

Critical point and mechanism of the phase transition in warm dense hydrogen

Ilnur Saitov[*1,2], **Genri Norman**[1,2]

[1] *National Research University Higher School of Economics (NRU HSE), Moscow, 101000, Russia*
[2] *Joint Institute for High Temperatures RAS, Moscow 125412, Russia*

The mechanism of the fluid-fluid phase transition in warm dense hydrogen is suggested and the corresponding critical point is estimated in the given work. The density functional theory is applied for the calculation of the equation of state, proton-proton pair correlation functions g(r) (PCF) and conductivity in the density and temperature range, where the phase transition is suggested. The results are averaged over the set of equilibrium ion configurations. The VASP plane-wave code is used.

The values of the PCFs first local maxima $g(r_{max1})$ and first local minima $g(r_{min1})$ are changed dramatically in the narrow density range of the expected phase transition, contrary to the ratio of the second maxima and minima $g(r_{max2})/g(r_{min2})$ which varies smoothly with the density. To emphasize the character of g(r) changes, the dependence of ratio $g(r_{max1})/ g(r_{min1})$ on density is considered. Jumps for T=2500 and 4000K are clear indications of the phase transition at the expected densities. The dependence of discontinuity of ratio $g(r_{max1})/ g(r_{min1})$ on temperature gives us the estimation of critical temperature T_c~4000K which is two times higher than the value of T_c predicted in [1] and agrees with recent measurements of Mochalov et al.

A two-step mechanism is suggested. The first stage is related to the partial ionization of H_2 molecules at the phase transition with formation of the molecular ions H_2^+. The second stage is a reaction of H_2 molecules and H_2^+ ions to form H_3^+ ions. The nature of the phase transition combines the ionization and the structure transformation. Strong ionization during the fluid-fluid phase transition in warm dense hydrogen distinguishes it from the liquid-liquid phase transitions [2]. An analogy can be found with the prediction [3], since the phase transition is due to ionization process. However, structural changes in [3] was not provided.

The work is supported by the Russian Academic Excellence Project '5-100'.

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* email: saitovilnur@gmail.com

Effect of quantum degeneracy on electron-atom scattering in partially ionized dense plasmas

S. M. Amirov [*1, 2], **T. S. Ramazanov** [1], **and Zh. A. Moldabekov** [1],

[1] *Institute of Experimental and Theoretical Physics, Al Farabi Kazakh National University, Almaty, Kazakhstan*
71 Al-Farabi ave., 050040 Almaty, Kazakhstan and
[2] *Institute of Applied Sciences and Information Technologies,*
40-48 Shashkin str., 050038 Almaty, Kazakhstan

The knowledge of electron-atom scattering processes is important for the description of dense partially ionized plasmas [1-3]. The main goal of this research is to analyse the importance of inclusion of the so-called quantum non-locality (difraction) effect into the description of screening of the polarised atom potential in partially ionized dense plasmas. The screened interaction potential between the charged particle and polarized atom in dense plasmas taking into account the electron degeneracy effect in random phase approximation was derived in Ref. [4]. On the basis of this potential the differential and total elastic scattering cross section, transport cross section, conductivity coefficient, and electron-atom collision frequency are calculated. Scattering phase is calculated via so-called Calogero equation [5].
The paper also presents the analysis based on the first order Born approximation and the eikonal method. It was found out that the modification of screening due to the quantum diffraction effect becomes important when the quantum degeneracy parameter (ratio of the thermal energy to the Fermi energy) is less than unity. In particular, the scattering phase shift can increase by 30 percent.

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* email: amirov.samat@gmail.com

The calculations of thermophysical properties of Ta plasma

Evgeny Apfelbaum[1*]

[1] *Joint Institute for High Temperatures of Russian Academy of Sciences, Izhorskaya str. 13 bldg. 2, Moscow 125412, Russia*

The thermophysical properties of substances (pressure, internal energy, conductivity etc.) are important in theory and applications. So they have been studied for more than a century. But the plasma region for metals is located at relatively high temperatures (T > 5000-10000 K), so it is less investigated in comparison with liquids and solids. It is the case in particular for tantalum plasma. Although there are corresponding data for various metallic and semiconductors plasmas [1], for Ta plasma analogous information is limited. In particular for Ta plasma there are experiments along release isoenthropes in shocks [2], conductivity measurements at constant energy input [3] and *ab initio* calculations of equation of state [4]. But excluding for conductivity measurements, these data are located at relatively high densities at $\rho > 2$ g/cm^3. (The density of Ta at ambient conditions is 16.69 g/cm^3, while the critical point is estimated as $T \sim 10^4$ K, $\rho \sim$ 4-5 g/cm^3 [4]).

Previously we have developed a model for calculations of thermodynamics and electronic transport coefficients for metallic plasma [5-7], which was successfully applied to different metals. The thermodynamics and composition were calculated within the chemical approach, when plasma is considered as a mixture of electrons, positive ions and atoms. For transport coefficients the relaxation-time approximation was used. In present report we have applied this model to Ta plasma and have estimated its region of applicability on the density-temperature plane. The comparisons with available experiments and calculations have shown good agreement within this region.

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[*] e-mail: apfel_e@mail.ru

Two-component plasma stopping power directly from partial static structure factors

A. Askaruly*[1], Yu.V. Arkhipov[1], A.B. Ashikbayeva[1], A.E. Davletov[1], D.Yu. Dubovtsev[1], S. Syzganbayeva[1], I.M. Tkachenko[2]

[1] Al-Farabi Kazakh National University, Almaty, Kazakhstan
[2] Universidad Politécnica de Valencia, Valencia, Spain

Reliable knowledge of energy losses of heavy projectiles is of substantial significance for the progress of inertial fusion and other practical applications. Polarizational stopping power of hydrogen-like dense plasmas

$$\left[-\frac{dE}{dx}\right]^{pol} = \frac{2\left(Z_p e\right)^2}{\pi\, v^2}\int_0^{\infty}\frac{dk}{k}\int_0^{kv}\omega^2 L(k,\omega)d\omega,$$

($Z_p e$ and v are the projectile charge and velocity) is studied within the moment approach which constructs the system loss function , $\varepsilon(k,\omega)$being the system dielectric function, in terms of only the system partial static structure factors so that $L(k,\omega)$ satisfies all convergent sum rules and other exact relations [1,2]. Electron-ion correlations in the target plasma are also taken into account [3] without using the simulation data. Enhancement of the stopping power is observed with respect to that in electron fluids [4], where the asymptotic values are always higher than the calculated ones, see Figure, for example.

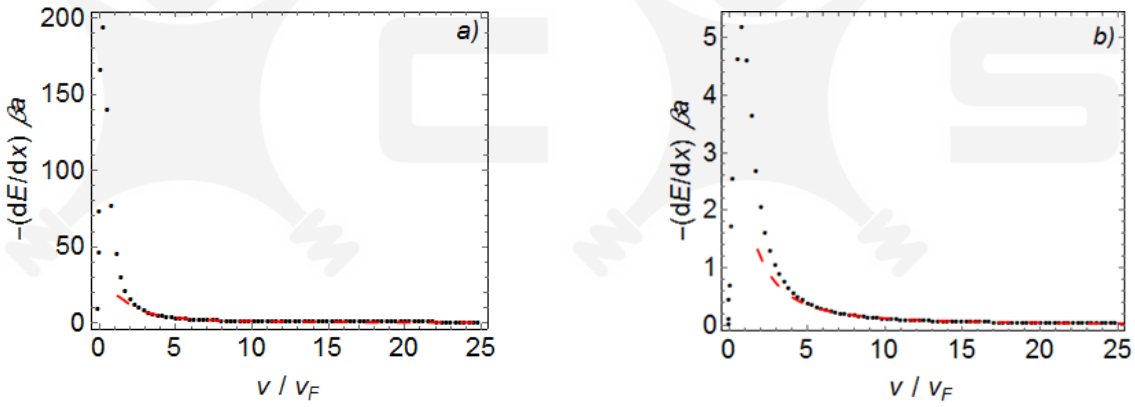

Figure: *Calculated stopping power (dots) and its asymptotic form (red dashed line) [3] at a) Γ= βe²/a = 10.77; b) Γ= 1.077, β^{-1}, a, and v_F are the plasma tempreature, electronic Wigner-Seitz radius and Fermi velocity, respectively. The structure factors were calculated in the hyper-netted chain approximation.*

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* email: abdiadil.askaruly@kaznu.kz

Ab initio simulations of the dynamic ion structure factor of warm dense lithium

B.B.L. Witte[*1,2], **M. Shihab**[3], **S.H. Glenzer**[2] **and R. Redmer**[1]

[1] Universität Rostock, Institut für Physik, Rostock, Germany
[2] SLAC National Accelerator Laboratory, Menlo Park, USA
[3] Tanta University, Department of Physics, Tanta, Egypt

We present molecular dynamics simulations based on finite-temperature density functional theory that determine self-consistently the dynamic ion structure factor and the electronic form factor in lithium. Our comprehensive data set allows for the calculation of the dispersion relation for collective excitations, the calculation of the sound velocity, and the determination of the ion feature from the total electronic form factor and the ion structure factor [1]. The results are compared with available experimental x-ray scattering and neutron scattering data. Good agreement is found for both the liquid metal and warm dense matter domain [2]. Finally, we study the impact of possible target inhomogeneities on x-ray scattering spectra.

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* email: bastian.witte@uni-rostock.de

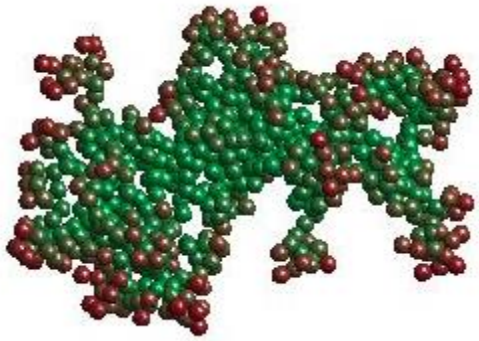
Effect of dust charging on turbulence in protoplanetary disks

K. S. Ashrafi*, S. Esparza, C. Xiang, A. Carballido, L. S. Matthews, and T. W. Hyde

Center for Astrophysics, Space Physics, and Engineering Research (CASPER), Baylor University, Waco, Texas, USA

Small dust grains are a major constituent of the material making up protoplanetary disks. In the earliest stages of planet formation, these grains agglomerate to form larger bodies, which are the precursors to planetesimals. Many protoplanetary disk models invoke turbulence produced by the magnetorotational instability (MRI) to provide the large relative velocities needed to allow the grains to agglomerate efficiently. The dust grains, however, collect electrons and ions from the gas and provide a surface for electron recombination. This changes the ionization fraction of the disk gases, affecting the coupling with magnetic fields which drives MRI turbulence. Thus a complete model of grain growth requires a feedback loop between the dust size and density, the disk opacity, the ionization of the gas, and resultant turbulence.

The collisional charging of a grain by the ambient plasma is affected by its surface area and morphology. In this work, we compare the electron and ion currents to micron and submicron grains which consist of aggregates of spherical monomers to those incident on spherical grains of equivalent mass. The electrons and ions are absorbed on the dust grain surface at random times; as a result charge fluctuates stochastically. We calculate the average charge and charge distribution for (i) aggregates composed of monomers of 10 nm, 20 nm and 50 nm monomers with an effective aggregate radius of 0.1 μm, and (ii) aggregates consisting of up to 50 monomers with monomer radius of 0.1 micron. The implications of our results for grain growth are briefly discussed.



* email: khandaker_ashrafi@baylor.edu

Coupling strength of two-dimensional dust clusters in anharmonic traps

A. Bessaa* and M. Djebli
Theoretical Physics Laboratory
U.S.T.H.B.; P.B.32 Bab-Ezzouar; 16079 Algiers, Algeria

Ordered structures are widely observed in dusty plasmas confined by a two-dimensional parabolic trap. The onion shell model in a finite system can be accurately reproduced with different packing structures by using a 2D Yukawa system in a power law trap. In order to characterize the structure of the resulting configurations, first-principle results from radial distribution function (RDF) are derived. With the data presented here, a matching between the structure, by means of RDF, and the coupling strength is possible.

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*email: abessaa@usthb.dz

Static and dynamic properties of finite-size dust particles in a plasma

Davletov A.E.*[1], Yerimbetova L.T.[1], Askaruly A.[1], Arkhipov Yu.V.[1], Tkachenko I.M.[2]

[1] Al-Farabi Kazakh National University, Science Research Institute of Experimental and Theoretical Physics, Almaty, Kazakhstan
[2] Universidad Politécnica de Valencia, Valencia, Spain

The study of the physics of dusty plasmas is one of the rapidly developing branches of modern plasma physics, since the presence of micron-sized particles results in a number of interesting phenomena. Mostly all of them emerge because those micron particles, called dust grains, readily acquire a fairly high electric charge in the plasma medium, which has a significant impact on the static and dynamic characteristics of the plasma.

This report specifically focuses on studying the static correlation functions (i.e. the radial distribution function and the static structure factor) of dust particles of finite dimensions that interact via the potential initially proposed in [1]. Treatment of the finite-size effects starts from the stage of dust electric charge evaluation within the orbital motion limited approximation, which leads to a significant change in the behavior of the static correlation functions. The radial distribution functions are iteratively calculated from the solution of the modified hyper-netted chain approximation proposed by Lado [2], which takes into account the inability of mutual penetration of the dust particles by incorporating the hard sphere potential. Thermodynamic properties of the dust component have been calculated and compared with the results of the available approximations and computer simulations.

The application of the method of moments has made it possible to elaborately investigate the electrodynamic characteristics of dusty plasmas; in particular, the dispersion and damping decrement of dust acoustic modes have been evaluated to demonstrate that the formation of the strongly decaying roton turns possible [3].

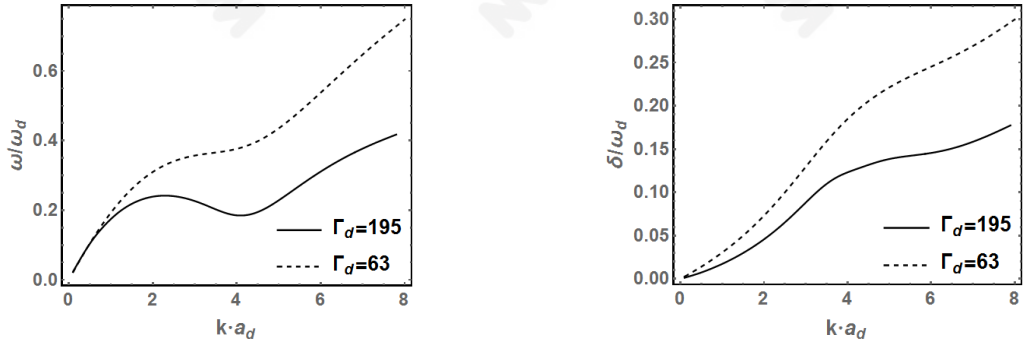

Figure: *Dispersion (left) and damping decrement (right) of dust acoustic modes against the dimensionless wavenumber with ad being the Wigner-Seitz radius for different values of the coupling parameter of dust particles*

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* email: askar@physics.kz

Using the Fluctuation Theorem in Strongly Coupled Plasmas

John Goree*, Chun-Shang Wong, Zach Haralson

Department of Physics and Astronomy, The University of Iowa, Iowa City, Iowa USA

The Fluctuation Theorem (not to be confused with the similarly named Fluctuation Dissipation Theorem) describes stochastic fluctuations in small nonequilibrium systems. This theorem has been used in various physical systems, such as large molecules or microspheres immersed in liquids. Until now, however, the literature for plasma physics has said little about this theorem.

We have conducted an experiment to demonstrate that the theorem is applicable to strongly coupled plasmas. The experiment was performed in a dusty plasma undergoing a shear flow. A dusty plasma is an ionized gas that contains, in addition to electrons and ions, micron-size solid particles that have large electric charges. The solid particles interact among themselves with a Coulomb repulsion large enough to provide strong coupling in a crystalline-like state. This crystal is then melted, using laser heating, to yield liquid-like conditions. Using video microscopy to track particle motion in a small subsystem, we observe fluctuations in the entropy production rate associated with viscous heating. These fluctuations are shown to agree with the Fluctuation Theorem.

Having demonstrated the applicability of the Fluctuation Theorem to strongly coupled plasmas, we can suggest that the theorem may find further use, for example in obtaining thermodynamic properties using simulations of a strongly coupled plasma, by observing small samples within the simulated volume.

Work supported by the U.S. Department of Energy and NASA.

* john-goree@uiowa.edu

Physics of wake structure in a flowing magnetized plasma

Sita Sundar[*1], Hanno Kaehlert[1], J.-P. Joost[1], Patrick Ludwig[1], and Michael Bonitz[1]

[1] *Christian-Albrechts-Universitaet zu Kiel Germany*

Dynamical screening and wake effects in complex plasmas have been the subject of many early investigations, including experimental [1] as well as theoretical work [2]. However, it was shown in experiments [3] and using Linear Response (LR) theory [4] that the characteristic features of the wake potential are qualitatively different in the presence of a magnetic field. Here, the electrostatic potential of a dust grain in a flowing magnetized plasma is computed using the 3D parallel PIC Code COPTIC [5]. In addition to the magnetic field, the system takes into account the effect of ion-neutral collisions. We compare our numerical results with the wake potential obtained from the LR formalism for magnetized as well as unmagnetized [6] cases. We discuss the physics of flux, distribution function etc. around the grain and present a parametric study of magnetization vs. wake peak position, peak potential etc. for the magnetized streaming plasmas.

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* email: sundar@physik.uni-kiel.de

Binary collisions in strongly coupled classical plasmas in the uniform magnetic field

N.Kh. Bastykova*, S.K. Kodanova, T.S. Ramazanov, Zh.A. Moldabekov

Institute of Experimental and Theoretical Physics, Al-Farabi Kazakh National University, Almaty, Kazakhstan

The influence of magnetic field on strongly coupled dusty plasmas has been the subject of close attention of plasma physicists over the last few years [1–3]. The knowledge of ion capture and scattering cross sections as well as transport properties of the magnetized non-ideal plasma is of high importance for astrophysics and for future inertial confintment fusion devices. Transport properties and ion-dust particle scattering cross section can be studied in the binary collision approximation [4-6]. Therefore, the binary collision between the ion and the dust particle is the subject of this paper.

In this work the scattering processes of charged particles around the dust particle in complex plasma in the presence of a strong uniform magnetic field are studied. The scattering angle and cross section of the binary collision of the ion with the dust particle have been obtained on the basis of ion trajectories around the dust particle. The trajectories of ions are calculated by the equation of motion using the Velocity Verlet Algorithm for strong external magnetic fields [7].

The results of this work will be used for calculation of the ion drag force and analysis of the dust particle charging in magnetized plasmas.

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* email: bastykova_nuriya@physics.kz

Momentum distribution functions of one and two component non-ideal quantum Coulomb systems

Filinov V.S.[1], Schoof, T.[2] Larkin A.S.[1,3], and Bonitz M.[2]

[1] Joint Institute for High Temperatures RAS, Moscow, Russia
[2] ITAP, CAU Kiel
[3] Moscow Institute of Physics and Tecnology, Dolgoprudny, Russia

In classical statistics the commutativity of kinetic and potential energy operators leads to the Maxwell distribution (MD) function, even for the strong interparticle interaction. In contrast, in quantum systems the interparticle interaction can affect the shape of the particle kinetic energy distribution function. Interactions restrict the volume of configuration space and, the Heisenberg uncertainty principle results in an increase of the occupied volume in momentum space, i.e., in a rise in the fraction of particles with higher momenta. Exchange effects, which lead in case of ideal particles to the Fermi-Dirac or Bose-Einstein distributions, may be also important under these conditions. On account of these effects the momentum distribution function of interacting fermions may contain a power-law tail even under conditions of thermodynamic equilibrium [1]. This effect may strongly influence chemical or nuclear reaction rates and may be important in studies of combustion, detonation and even nuclear fusion.

Under extreme conditions systems of particles are usually strongly coupled and perturbative approaches are not applicable.Therefore, for the calculation of the momentum distribution *ab initio* non-perturbative methods are required. In this work we consider one and two-component non – ideal Coulomb systems and use two ab initio and two approximate quantum Monte Carlo (QMC) approaches that we recently developed and compare the obtained results.

In the first approximate approach, to obtain explicit expressions for the Wigner function we use linear or harmonic local approximations for the interparticle potential [2] and take into account Pauli blocking of fermions by pair effective exchange pseudopotential depending on coordinates, momentum and parameter degeneracy. The second approximate method (single-momentum) is based on the reduced Wigner functions, integrated over all momenta except several few.

The first ab inito approach (configuration path integral Monte Carlo, CPIMC) is based on representation of the N-particle density operator in a basis of (anti-)symmetrized N-particle states [3]. The main idea of this approach is to evaluate the path integral in space of occupation numbers instead of configuration space. In the second ab initio approach the Monte Carlo simulations are carried out by permutation blocking path integral Monte Carlo (PB-PIMC) [4]. To simulate fermions in the canonical ensemble, it was combined with a fourth-order approximation of the density matrix derived with a full anti-symmetrization on all time slices.

In our results we concentrate on the "power law tails" predicted by [1], compare them to our QMC results and study their dependence on the plasma parameters.

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Quantum tails in momentum distribution functions of non-ideal Fermi systems.

Larkin A.S.[1,2], **Filinov V.S.**[1]

[1] *Joint Institute for High Temperatures RAS, Moscow, Russia*
[2] *Moscow Institute of Physics and Tecnology, Dolgoprudny, Russia*

Quantum effects may affect equilibrium momentum distribution functions making them non-maxwellian. For example, exchange effects lead to Fermi-Dirac or Bose-Einstein distributions in systems of non-interacting particles. On the other hand, interaction between particles restricts available for particle volume and could result in broadening of momentum distribution due to Heisenberg principle. This effect may strongly influence the reaction rates and may be important in studies of combustion, detonation and even nuclear fusion [1]. Under extreme conditions systems of particles are usually strongly coupled and perturbative approaches are not applicable. Therefore *ab initio* non-perturbative methods for calculation of momentum distribution functions are required.
In this work we use path integral representation for Wigner function [2] and propose two Monte Carlo methods for studies of momentum distribution functions of degenerate non-ideal Fermi systems. In the first method to obtain explicit expressions for Wigner functions we take into account *pair exchange* interaction of fermions and *linear* or *harmonic* local *approximations of interparticle potential. The second method (single-momentum) is based on reduced Wigner function, integrated over all momenta except several few.*
Both methods have been tested on simple models: one particle in different external potential fields and ideal Fermi gas (see figure: left plot). Results are in good agreement with available analytical and numerical data. Then momentum distribution functions for a two component degenerate plasma media have been investigated. Quantum corrections to Fermi and Maxwell distributions in form of "power tails" predicted by [1] have been found (see figure: right plot). This work has been supported by the Russian Science Foundation via grant 14-50-00124.

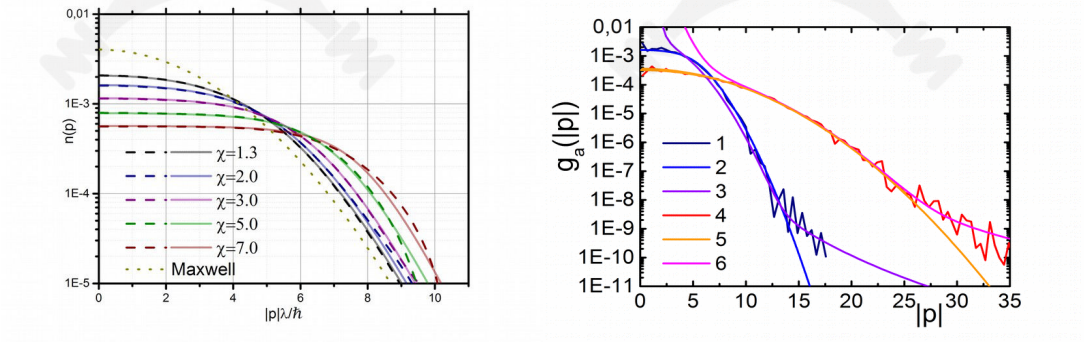

Figure: *Left plot: momentum distributions for ideal Fermi gas calculated by proposed single-momentum Monte Carlo method (solid lines) and analytical Fermi distributions (dashed lines) for different parameters of degeneracy. Right plot: momentum distributions for non – ideal plasma of electrons (lines 1,2,3) and five times heavier holes (lines 4,5,6); MC results – 1,4; Fermi distributions - 2,5; "power tails $1/p^8$" - 3,6; degeneracy of electrons is equal to 2.5, plasma coupling parameter – 1.*

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Ab initio approach to ion stopping at the plasma-solid interface

Karsten Balzer[*1], **Niclas Schlünzen**[2], **Jan-Phlip Joost**[2], **Lasse Wulff**[2], **Michael Bonitz**[2]

[1] *Computing Center, Christian-Albrechts-Universität zu Kiel, Ludewig-Meyn-Str. 4, 24118 Kiel, Germany*
[2] *Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel, Leibnizstr. 15, 24098 Kiel, Germany*

The energy loss of ions in solids is of key relevance for many applications of plasmas, ranging from plasma technology to fusion. Standard approaches are based on density functional theory or SRIM simulations, however, the applicability range and accuracy of these results are difficult to assess, in particular, for low energies. Here, we present an independent approach that is based on *ab initio* nonequilibrium Green functions theory, e.g. [1,2] that allows to incorporate electronic correlation effects of the solid. As a first application of this method to low-temperature plasmas, we concentrate on proton and alpha-particle stopping in a graphene layer and similar finite honeycomb lattice systems. In addition to the stopping power we present time-dependent results for the local electron density, the spectral function and the photoemission spectrum [3] that is accessible in optical, UV or x-ray diagnostics [4].

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* email: balzer@rz.uni-kiel.de

Theoretical approach to the interaction of plasmas with strongly correlated materials

M. Bonitz[*1], K. Balzer[2], H. Kählert[3], A. Filinov[1,3], E. Pehlke[1], and B. Hartke[4]

[1] *Institut für Theoretische Physik und Astrophysik, CAU Kiel, Germany*
[2] *Rechenzentrum, CAU Kiel, Germany*
[3] *INP Greifswald, Germany*
[4] *Institut für Physikalische Chemie, Germany*

The interaction of low-temperature plasmas with solid surfaces is of crucial importance for many technological applications. There exist many successful applications of these plasmas, however, most of them are being discovered in a trial and error manner. A new research initiative in Kiel aims at developing a fundamentally different approach that is based on first-principle simulations. Here we present an overview on our theoretical concept that is based on a combination of ab initio Time-dependent Density Functional Theory simulations, reactive force fields and molecular dynamics and kinetic Monte Carlo simulations. Moreover we present a strategy for an integrated nonequilibrium quantum kinetic approach to the plasma-solid interface that is based on nonequilibrium Green functions and couples to a particle in cell-Monte Carlo collision simulation of the plasma.

* email: bonitz@theo-physik.uni-kiel.de

Microscopic modelling of Ar scattering from Au and Pt (111/100) surfaces

A. Filinov[*1,2,3], **M. Bonitz**[1], **D. Loffhagen**[2]

[1] *Institut für Theoretische Physik und Astrophysik, CAU Kiel, Leibnizstr. 15, D-24098 Kiel, Germany*
[2] *INP Greifswald e.V., Felix-Hausdorff-Straße 2, 17489 Greifswald, Germany*
[3] *Joint Institute for High Temperatures RAS, Izhorskaya Str. 13, 125412 Moscow, Russia*

The investigation of structure and dynamical properties of surfaces using atomic probes as scattering projectiles has proven to be a useful experimental tool. The scattered intensity as a function of final translational energy, scattered and incident angles is measured and provides an important information on surface corrugation and temperature effects. For a strongly corrugated surface a target can be considered as a collection of discrete scattering centers, while in the opposite limit scattering is treated as a single impulsive collision with a smooth surface when the main dissipation channel is the excitation of surface phonon modes. The efficiency of the gas-lattice energy exchange can be related to the gas-to-lattice mass ratio, the depth of physisorption potential well and the surface corrugation.
Both regimes can be distinguished by analyzing a temperature-dependence of the scattered intensities, and the probabilities of direct inelastic scattering and trapping-desorption processes.

Our main goal is to provide a detailed analysis via a direct simulation of atom-surface collisions by using two approaches: molecular dynamics (MD) simulation and a stochastic scattering theory based on the reconstructed differential reflection coefficient. The gas-surface interactions are treated via the effective pair potential determined from the non-local van-der-Waals approach [1]. Different energy dissipation channels in the adsorption process are included. The electron-hole pair excitations are considered via the model of electronic friction [2]. The phonon excitations are treated via the Langevin MD simulations.

For the scattering of argon atoms on surface of aurum and platinum first results have been obtained for the direct scattering fraction and the sticking coefficient. The energy and angular distributions of the scattered particles are resolved as a function of the incident energy, the incident angle and the lattice temperature. Following the multiple collisions on the trapped fraction we also determined the average trapping time, the desorption probability and how an enclosed gas comes to equilibrium with the surface.

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* email: filinov@theo-physik.uni-kiel.de

Dielectric response function for warm dense matter states

Kushal Ramakrishna[1], **Jan Vorberger**[1]
[1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

The dynamic structure factor (DSF) is an important parameter to determine warm dense matter properties and can be accessed using x-ray Thomson scattering from energetic x-ray sources at LCLS, SACLA or EU-XFEL[1,2]. To improve upon the existing DSF models with greater accuracy and better description to model high pressure solids and liquids, a good agreement between theory and experiment is needed taking into account the electron-hole interaction resulting from an optical absorption, especially if the system is a semiconductor or an insulator. In a theoretical framework, we need access to the dielectric response function calculated using methods such as RPA, GW or even BSE based on density functional theory[3,4]. Small-gap semiconductors and metals, instead, screen this electron-hole interaction, and the resulting contribution can therefore be negligible. The Bethe-Salpeter equation indeed couples the electron and the hole, and has been very successful for the calculation of absorption spectra of a large variety of systems: insulators, semiconductors, atoms, clusters. We would like to present the results using aforementioned methods for different systems modelling warm dense matter states.

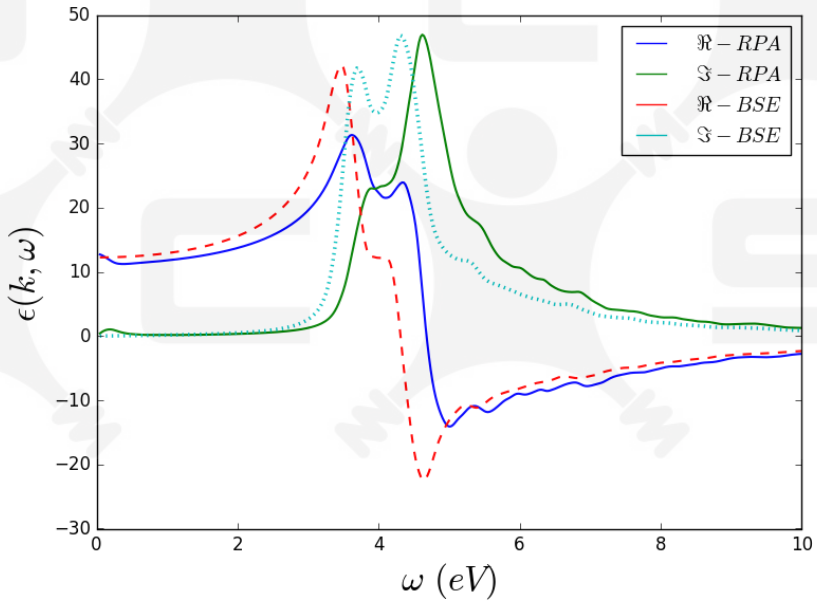

Figure 1: Dielectric function for Silicon

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[1]email:k.ramakrishna@hzdr.de

Excitation of electron pulse-driven wakefields in metallic nanostructures

Shabbir A. Khan[*1]

[1] *National Center of Physics, Quaid-i-Azam University Campus, Islamabad 45320, Pakistan*

Taking into account the dispersive dielectric response of nanostructures, we study the excitation of electrostatic wakefields in mettalic nanowires as a result of propagating short electron pulse. In the context of spatially nonlocal response of the system, existence and stability conditions of electrostatic wakefields are discussed theoretically and the role of exchange-correlation effects in local density applroximation is highlighted for typical data of Au nanowires. Inclusion of the exchange-correlation potential in the model generalizes the results as compared to previous studies in literature. The stability conditions of the wakefields indicate that the underlying mechanism can be useful in the wakefield excitation in nanowire as a narrow source of radiation in the extreme ultravoilet frequency range.

* email: sakhan@ncp.edu.pk

Simulation of metal cluster growth on a thin polymer film during sputter deposition

J. W. Abraham[*1], **T. Strunskus**[2], **F. Faupel**[2], **M. Bonitz**[1]

[1] *Institut für Theoretische Physik und Astrophysik, University of Kiel, Germany*
[2] *Institut für Materialwissenschaft, University of Kiel, Germany*

The fabrication of metal-polymer nanocomposites with tailored optoelectronic properties has been a challenge since the early days of nanotechnology. Under typical conditions in plasma-based physical vapor deposition experiments, crucial properties such as composition, size and shape of the nanoparticles evolve in a self-organized process and are hence difficult to obtain in a controlled way.

Computer simulations can be helpful to improve the understanding of the relevant processes, but the required length and time scales impose big challenges on all currently available methods. In this work, we present an approach based on Langevin dynamics that allows us to investigate the growth of gold and bi-metallic Ag-Cu clusters on polymer surfaces on experimentally relevant time scales [1]. The method takes into account the deposition of single metal atoms, diffusion of the particles on the surface, desorption of atoms as well the creation of surface defects caused by the impingement of ions that are emitted from the plasma environment. We show that our results are in good agreement with recent GISAXS experiments that were carried out to study the morphology and optical properties of sputtered gold on a thin polystyrene film in real time [2]. Finally, we demonstrate some approaches to calculate the intensity of scattered X-rays as well as the UV-Vis absorption spectrum for our simulated structures.

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* email: abraham@theo-physik.uni-kiel.de

Nonlinear effects in a weakly ionized gas exposed to a strong shock wave

Triaskin J.V.[*1], **Pavlov V.A.**[1]

[1] *Physics Department, St. Petersburg State University, 1, Ulyanovskaya str., Petrodvorets, 198504, St. Petersburg, Russia*

The interaction of neutral and charged gas components is in a high interest. This attention is caused mostly by aerospace applications as well as for exploring the nonlinear wave processes in the near-Earth space. In this work, the interaction of strong shock waves and supersonic bodies with low-ionized plasma is presented and discussed.

A motivation to the study is the discovery of the effect of anomalous supersonic flow of low-ionized plasma around a body in the absence of energy release ahead of the body [1]. Later, anomalous relaxation and instability of shock waves in gases were found in [2]. Generation of low-ionized gas-discharge non-isothermal plasma ahead of a body, streamlined by a supersonic flow, allows lowering the intensity of a strong shock wave [3]; this effect reduces the aerodynamic drag.

The essence of the phenomenon is the formation of a region with elevated concentration of charged particles ahead of the front of a shock wave at certain speed of the latter. This critical speed is defined by the electron temperature and ion mass. Laboratory experiments show the flow around a body by weakly ionized air to differ markedly from that by heated neutral air. The 'plasma effect' is manifested in distancing of the head shock wave from the body and lowering of its intensity.

Under certain conditions, total 'destruction' of a shock wave is possible due to the presence of gas ionization ahead of the body. Analytical studies assumed rather far-reaching idealizations. Based on computer simulation [4], formation of a plasma precursor was shown to be possible ahead of the shock wave front – a soliton with a critical property: a non-monotonic resonant dependence of the soliton amplitude on the shock wave speed. The maximum perturbations develop at values of the shock wave speed in the range $c \approx (1.6 \div 2) u_s$, (u_s is the ion sound speed).

In such situation, a sole, densest possible, local condensation of charged particles is formed in the precursor. The gas in the 'condensation' is not weakly ionized anymore, and charged particles can exert a reciprocal effect upon the neutral component and the shock wave. The 'competition' between strong nonlinearity and strong dispersion causes appearing of a sharp decrease of the soliton amplitude with the shock wave speed growing beyond critical value c. Previously similar effect have been found in [5] in hydrodynamic and called 'Houston's horse' effect.

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* email: jaroslav.triaskin@spbu.ru

Correlation-induced second plasmon in an electron liquid

Gabor J. Kalman[1], Kenneth I. Golden[2], Luciano Silvestri[1*]

[1]*Department of Physics, Boston College, Chestnut Hill, Massachusetts, 02467, USA*
[2]*Department of Mathematics & Statistics & Dept. of Physics, University of Vermont, Burlington, VT 05405, USA*

Based on recent analytic and Molecular Dynamics simulation results pertaining to binary systems we predict the existence of a second, low, but finite frequency plasmon in a strongly coupled 3D electron liquid at zero temperature. This excitation is maintained by the out-of-phase oscillations of the spin-up and spin-down densities of the electron liquid, but governed solely by the Coulomb interaction between the particles. The frequency square of this mode is proportional to the overlap ($r = 0$) (absolute) value of the spin-up/spin-down pair correlation function, and is thus only slightly affected by the degree of polarization of the electron liquid. We estimate the spectral weight of the mode, based on the assumption that interspecies viscous drag is the principal mechanism for damping in the strong coupling domain. The spectral weight is manifest in the partial spin-resolved dynamical structure functions and it is proportional to the product of the two densities of the spin components. The connection with recent discussions concerning spin resolved structure functions for the electron liquid [1] is explored. It is pointed out that a scattering experiment with circularly polarized neutrons [2] or circularly polarized X-rays [3] may be a possible avenue to observe equilibrium fluctuations associated with this excitation. This research has been supported by NSF

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* silveslu@bc.edu

The effect of spin-orbit interaction on structural stability and thermodynamic properties of lead under pressure

Nikolai Smirnov*

Russian Federal Nuclear Center — Institute of Technical Physics, Snezhinsk, Russia

The effect of spin-orbit (SO) interaction on lead properties under pressure is investigated through calculations by the FP-LMTO method [1] which determines the band structure of crystals from first-principles. The calculations are done in generalized gradient approximation with the exchange-correlation functional PBEsol [2]. Relative specific volumes in the range V/V_0=1.05 – 0.45 are considered. The evolution of the band structure of lead with increasing crystal compression is studied. Calculated results include elastic constants, phonon spectra and compression curves for *fcc*, *bcc* and *hcp* lead. The calculations show that SO interaction weakly influences the 0K-isotherms which differ by no more than 2% at maximal compression among those considered. However, the phonon spectra obtained with and without SO interaction markedly differ at moderate compressions. For some frequencies, the difference reaches 25%. But it gets smaller as pressure grows and at *P*>200 GPa becomes faintly discernible approaching the limiting error of the calculation method used.

The effect of SO interaction on the structural stability of *fcc*, *bcc* and *hcp* Pb under pressure is also investigated. Calculated results are compared with various experimental data.

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* email: deldavis@mail.ru

Multicomponent electron-hole superfluidity and BCS-BEC crossover in double bilayer graphene

Sara Conti[*1,2], **David Neilson**[1], **Andrea Perali**[3], **Francois Peeters**[2]

[1] *University of Camerino, Camerino, Italy*
[2] *CMT, University of Antwerp, Antwerp, Belgium*

Superfluidity in coupled electron-hole sheets of bilayer graphene is multicomponent because of the conduction and valence bands[1]. We investigate the superfluid crossover properties as functions of the equal electron and hole densities and the tunable energy gap between the bands[3]. We determine the momentum dependent multicomponent superfluid gaps, the multicomponent condensate fractions, and the chemical potential. We find that interaction driven excitations from the valence band to the conduction band can block the system from entering the BEC regime even at very low densities.

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* email: sara.conti@uantwerpen.be, sara.conti@unicam.it

Interparticle / Interchain Forces in Field-Aligned Chains within a Complex Plasma

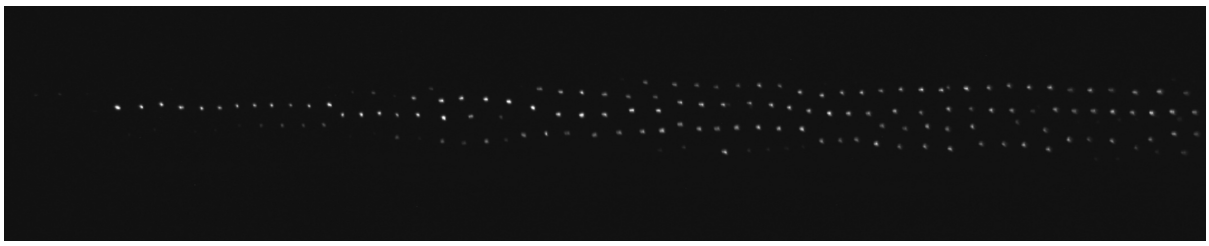
Truell W. Hyde*[1], Lorin Matthews[1], Peter Hartmann[1,2], Oleg Petrov[1,3], Vladimir Nosenko[1,4], Marlene Rosenberg[5], Jie Kong[1], Ke Qiao[1]

[1] *Center for Astrophysics, Space Physics and Engineering Research (CASPER), Baylor University, Waco, Texas, USA*
[2] *Wigner Research Centre for Physics, Budapest, Hungary*
[3] *Joint Institute for High Temperatures, Russian Academy of Sciences*
[4] *German Aerospace Center (DLR)*
[5] *University of California at San Diego*

In 1934 Wigner predicted theoretically that a gas of electrons, in which the kinetic energy (temperature) was comparable to the average potential energy, would form a symmetric lattice (i.e., a crystalline phase) at some critical value of the ratio of these energies. Since this time, various Wigner structures have been observed experimentally on Earth. To date, most have assembled under the presence of external system confinement, making the fundamental physics behind these correlation driven effects surprisingly difficult to determine.

Complex plasmas have proven to be a versatile analog for the study of such systems, particularly those where their global behavior is determined by the combined effect of the particles' low temperature / kinetic energy, interparticle / interchain interactions, global and/or local confinement and streaming ion flow. Of these, the ion wakefield force directly influences the interaction between the particles but is in general much weaker than other system forces. As such, its effects are often masked by gravity for terrestrial experiments.

In this talk, the role the ion wakefield plays in extended particle chain formation will be discussed for both gravitational and microgravity environments. A recently funded (NASA / NSF) project proposing examination of field-aligned chains formed in the PK-4, where the ion flow and resulting interparticle potential can be controlled by tuning an alternating DC bias, will also be discussed. Finally, it will be shown that thermally excited waves propagating along and perpendicular to such chains can provide details of the resulting interparticle / interchain potential allowing study of the relationship between this potential, the ion wakefield and the controlling DC bias.



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*email: Truell_Hyde@baylor.edu

Strong Coupling Corrections to Electron-Ion Collision Rates in Ultracold Plasmas

Jacob L. Roberts[*1], **Wei-Ting Chen**[1], **Craig Witte**[1]

[1] *Department of Physics, Colorado State University, USA*

In an ultracold plasma, an electron oscillation can be initiated via a short electric field pulse, causing the electrons to oscillate with respect to the ions. Under accessible experimental conditions, the damping rate of this oscillation is determined by the electron-ion collision rate. We have measured such an oscillation damping rate for an ultracold plasma with an electron strong coupling parameter of 0.35. The measured damping rate is far in excess of that predicted using a weak-coupling expression for the electron-ion collision rate. Our results are in good agreement with a molecular dynamics model of our system. However, our results are not in good agreement with a Monte Carlo-based random binary collision simulation, even if typical extensions to accommodate strong coupling are incorporated into the predicted electron-ion collision rate. The implications of and possible reasons for such a discrepancy will be presented.

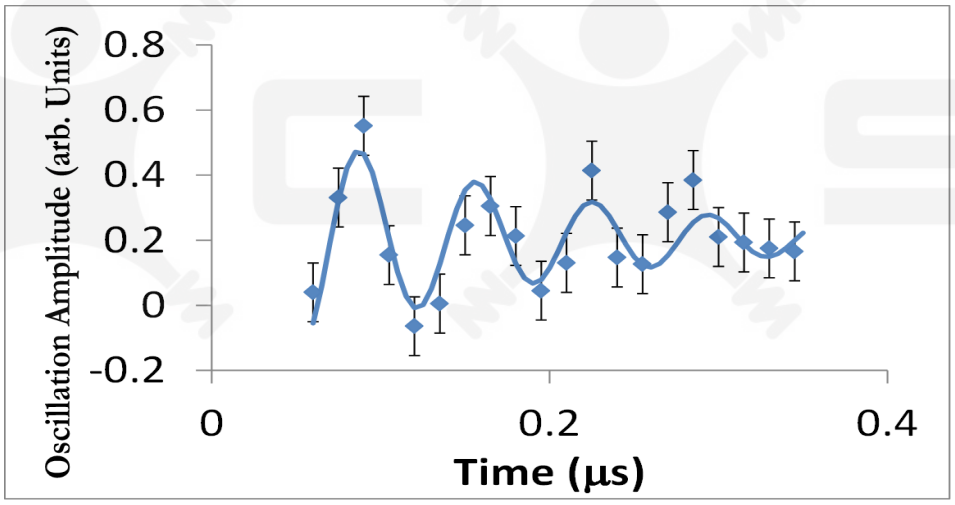

Figure: *Electron center-of-mass oscillation amplitude as a function of time after a sharp electric field pulse. These data were taken under experimental conditions where the damping rate is predicted to be dominated by electron-ion collisions, and so this data allows the determination of the electron-ion collision rate under the given experimental conditions.*

* email: Jacob.Roberts@colostate.edu

Structure of a Coulomb cluster in the cusp magnetic trap under microgravity conditions

L.G. Dyachkov*[1], T.S. Ramazanov[2], O.F. Petrov[1], M.M. Vasiliev[1], M.I. Myasnikov[1], V.E. Fortov[1], K.N. Dzhumagulova[2], M.T. Gabdullin[2], M.K. Dosbolayev[2], Y.A. Ussenov[2], Zh.A. Moldabekov[2], S.F. Savin[3], T.A. Musabaev[4], Zh.Sh. Zhantayev[4], A.A. Aimbetov[4]

[1]*Joint Institute for High Temperatures, RAS, Moscow, Russia*
[2]*Al-Farabi Kazakh National University, Almaty, Kazakhstan*
[3]*S.P. Korolev Rocket-Space Corporation "Energy", Korolev, Moscow region, Russia*
[4]*National Center of Space Research and Technology, KazCosmos, Almaty, Kazakhstan*

Experiment "Coulomb crystal" is performed under microgravity conditions aboard the International Space Station [1-3]. We study the properties of SCCS formed by diamagnetic (graphite) dust particles in a cusp magnetic trap. The cusp magnetic field is generated by two coils placed on the same axis, in which currents circulate in the opposite directions. Between the coils we have a potential well for diamagnetic particles where graphite particles are placed within a cylindrical glassy cell filled with argon at atmospheric pressure and room temperature. Particle charging is carried out using a central wire electrode passing along the cell axis. Here we discuss results of the last experiment [3] in which the cluster was formed by ~3×10^4 initially uncharged 300 μm particles and then its charging was carried out gradually increasing the central electrode potential up to 150 V in four steps by 37.5 V each with an interval of about 15 s. During three steps (45 s) the cluster lost about half of the particles in the form of the filamentary complexes. On the 3rd step (112.5 V) we see also small number of individual particles with velocities less than 1 cm/s. On the 4th step (150 V) the cluster is destroyed completely during 8 s, particles left the cluster surface mostly individually with velocities of 1 to 4.5 cm/s. We have calculated the relation between particle charge and velocity for each step, and based on observations and estimates, we can make some assumptions about the cluster structure. Features of particle scattering indicate that the cluster charge is located on its surface, therefore the cluster is conductive. The particle velocity spectrum points out a significant difference in their charges. Consequently, the surface is not completely conductive. Besides, the cluster structure is not compact: the particles occupy only about 10% of its volume. Apparently the cluster consists mainly of filamentary complexes, observed at the beginning of its destruction. They were formed, obviously, before the electrode potential was turned on. And they are oriented mainly from the center to the surface.

The work was supported by a grant of the RSF No. 14-50-00124.

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* email: dyachk@mail.ru

Function of state for Coulomb system in electrodynamic trap

Lapitsky D.S.[*1], **Filinov V.S.**[1]

[1] *Joint Institute for High Temperatures of the Russian Academy of Sciences, Moscow, Russia*

The paper presents the results of calculation of function of state of Coulomb systems. Coulomb systems of similarly charged particles are unstable and in this work the systems are retained in alternating electric fields of a quadrupole type of linear Paul trap. Simulation of charged micron sized similarly charged particles in alternating electric fields in air were carried out [1]. Using microscopic theory of disordered condense matter [2] the analysis of stable oscillating system were provided and the functions of state for Coulomb system were found, such as internal energy *U* in figure 1. The coulomb system is forced by external electric fields of the trap and oscillates. So in addition to thermal energy coulomb system is described also by mechanical energy *M* (kinetic and potential energy of particles). The comparison of internal energy *U* with the mechanical *M* and thermal energy indicated strongly coupled system. Figure 1 presents the coulomb system after 0.3 s after its injection in the trap and figure 2 presents the evolution of energy. It decreases to a certain value due to rather small interparticle distances while injection and fluctuates due to the influence of alternating electric field.

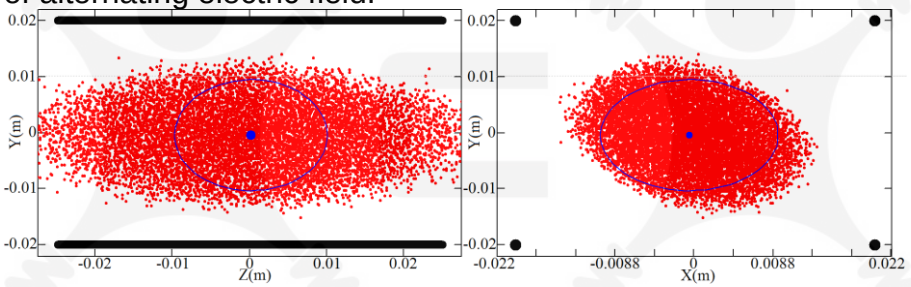

Figure 1: *Coulomb system of 10000 similarly charged 2 micron sized particles (red dots) with charges 11000 e in the trap. Left picture is side view, right one is end view. Black lines and dots correspond to trap electrodes. The blue ring indicates the region where the energy and pressure are calculated.*

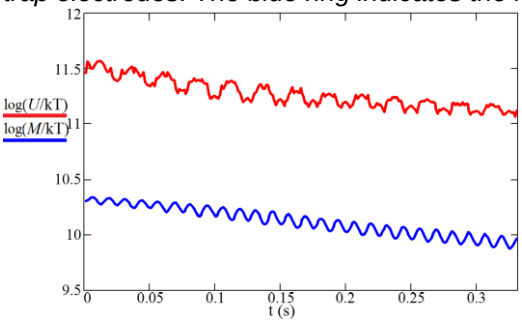

Figure 2: *Evolution of internal energy U and mechanical energy M.*

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* email: dmitrucho@yandex.ru

Strongly coupled complex plasma in a 2D harmonic trap

Hong Pan*[1], Peter Hartmann[1, 2], Zoltan Donko[1, 2], Gabor J. Kalman[1], Marlene Rosenberg[3]

[1] *Department of Physics, Boston College, Chestnut Hill, Massachusetts, 02467, USA*
[2] *Institute for Solid State Physics, Wigner Research Centre for Physics, Hungarian Academy of Sciences, H-1525 Budapest, P.O. Box 49, Hungary*
[3] *Department of Electrical and Computer Engineering, University of California, San Diego, La Jolla, CA 92093-0407, USA*

All "2- dimensional" complex (dusty) plasma layers are in effect only quasi 2-dimensional [1], since they have a finite thickness, whose size is determined by the strength of the confining electrostatic trapping potential. The density profile and structure of such systems has been the subject of a number of recent works [2, 3, 4, 5, 6], most of which have focused only on simulations. In the present work we use the YOCP (Yukawa One-Component Plasma) model to describe the dusty plasma and provide a theoretical analysis based on the HNC approximation to obtain the density profile in a harmonic trap. Both the liquid and solid phases are considered. The analytic work is accompanied by detailed MD simulations. The formation of the density profile is controlled by the screening parameter κ, the coupling strength Γ and the trap strength. When Γ is high enough, the plasma crystalizes, but the details of the liquid-solid phase boundary depend on all the parameters. As the trap strength is relaxed, the plasma splits into more and more layers. The number of layers is determined by the trap strength and kappa only, and for a given total layer width we can predict the number of layers. The 2D pair correlation function for liquid density profile has been analyzed. These latter are provided by high quality MD simulations, which also provide density profiles for comparison with the theoretical results. We also determine the phase boundary between the liquid and solid phases through various approaches. One can observe the remarkable effect of the trapping strength on the phase structure.

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CREDITS: OTKA, NSF

* email: hongpb@bc.edu

The affect of the strong magnetic field on the dusty plasma in dc discharge

Pavlov S. I.*, Karasev V. Yu., Dzlieva E. S.

St. Petersburg State University, St. Petersburg, Universitetskaya nab. 7/9, 199034, Russia

The role of the magnetic field in the creation and study of plasma was defined more than half a century ago. The role of the magnetic field for the complex plasma which was discovered 20 years ago is only to be clarified [1 – 4]. In existing works devoted to investigation of the complex plasma in strong magnetic field [5 – 7] only the rf discharge was used to create the dust trap. For example, the authors of [5] speak about an attempt and a refusal of using the dc discharge for the given problem.
In the present report the first results of the creation and observation of dusty plasma formed in the glow discharge in traps in the striation and in the area of the narrowing of the current channel. The existence of dusty plasma in the glow discharge in magnetic field of more than 1 T is experimentally shown.
To create the magnetic field the cryomagnet was used. For creation of the glow discharge the various discharge tubes were used. The tubes were filled with the neon at the pressure in the range from 0.3 to 0.9 Torr. Polydisperse quartz with a characteristic size of 5 μm was used as the dust particles. Several variants of cathodes were used which provide the stable discharge depending on the conditions and the magnitude of the magnetic field.
As the results, the dependences of the angular velocity of the dust structures rotations on magnetic induction and the arrangement of particles in the horizontal sections of the dust structure are presented.
The work is supported by the grant of the RSF No. 17-72-20006.

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* email: s.i.pavlov@spbu.ru, plasmadust@yandex.ru

Phase transitions in local approximation and anomalies of spatial charge profiles in non-uniform plasma thermoelectrostatics

Chigvintsev A Yu*[1], **Zorina I G**[2], **Noginova L Yu**[3] **and Iosilevskiy I L**[1,4]

[1] *Moscow Institute of Physics and Technology, Institutskiy Pereulok 9,Dolgoprudny, Moscow Region 141700, Russia*
[2] *Bauman Moscow State Technical University, 2nd Baumanskaya Street 5, Moscow 105005, Russia*
[3] *Russian State Agrarian University—Timiryazev Moscow Agricultural Academy, Timiryazevskaya 49, Moscow 127550, Russia*
[4] *Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia*

The “jellium” approximation i.e. replacing system of discrete particles (electrons and/or ions) by hypothetical “fluid” with pure local properties (i.e. depending on local density only) is widely used not only in hydrodynamic applications but in thermoelectrostatics i.e. in calculation of equilibrium charged particles distribution near a source of non-uniformity. The equation of state (EOS) that connects local pressure, energy and chemical potential of charged particles with local density and temperature, is used for this purpose (LDA approximation). In most cases it is ideal-gas (correlationless) approximations (i.e. Thomas–Fermi or Poisson–Boltzmann). The main problem of this approach is correct taking into account of mean-particle correlations (non-ideality). We provide calculations and discuss the results for charged particle equilibrium distribution in case when we use exact non-ideal EOS for one-component electronic or ionic systems with phase transitions included in such non-ideal EOS. The main result of such using of non-ideal EOS is appearance of phase transition-like discontinuities in equilibrium spatial profiles of non-uniform charge distribution at low enough (subcritical) temperatures. Features and parameters of these discontinuities are discussed and illustrated.

The work was supported by the Russian Scientific Foundation (grant 14-50-00124).

*email: alex012008@gmail.com

Influence of non-isothermality effect of plasma on Hugoniot adiabat

T.N. Ismagambetova[1], M.T. Gabdullin[2], T.S. Ramazanov[1]

[1] IETP, Al-Farabi Kazakh National University, 71, al-Farabi str., Almaty, Kazakhstan
[2] NNLOT, Al-Farabi Kazakh National University, 71, al-Farabi str., Almaty, Kazakhstan

In this work dense non-ideal, non-isothermal hydrogen plasma was considered. Effective screened interaction potentials taking into account the quantum-mechanical effect of diffraction were used [1]:

$$\Phi_{\alpha\beta}(r)=\frac{Z_\alpha Z_\beta e^2}{r}\frac{1}{\gamma^2\sqrt{1-\left(2k_D/\lambda_{ee}\gamma^2\right)^2}}\left(\left(\frac{1/\lambda_{ee}^2-B^2}{1-B^2\lambda_{\alpha\beta}^2}\right)\exp(-Br)-\left(\frac{1/\lambda_{ee}^2-A^2}{1-A^2\lambda_{\alpha\beta}^2}\right)\exp(-Ar)\right)-$$

$$-\frac{Z_\alpha Z_\beta e^2}{r}\frac{(1-\delta_{\alpha\beta})}{1+C_{\alpha\beta}}\exp(-r/\lambda_{\alpha\beta}), \qquad (1)$$

where α,β are types of particles, $\lambda_{\alpha\beta}=\hbar/\sqrt{4\pi\, m_{\alpha\beta}k_B T_{\alpha\beta}}$ is thermal de-Broglie wavelength, $T_{\alpha\beta}=\sqrt{T_\alpha T_\beta}$ [2], $m_{\alpha\beta}=m_\alpha m_\beta/(m_\alpha+m_\beta)$, $k_D^2=k_e^2+k_i^2$ is the screening parameter taking into account the contribution of electrons and ions, $\gamma^2=k_i^2+1/\lambda_{ee}^2$,

$$A^2=\frac{\gamma^2}{2}\left(1+\sqrt{1-\left(\frac{2k_D}{\lambda_{ee}\gamma^2}\right)^2}\right),\ B^2=\frac{\gamma^2}{2}\left(1-\sqrt{1-\left(\frac{2k_D}{\lambda_{ee}\gamma^2}\right)^2}\right),\ C_{\alpha\beta}=\frac{k_D^2\lambda_{\alpha\beta}^2-k_i^2\lambda_{ee}^2}{\lambda_{ee}^2/\lambda_{\alpha\beta}^2-1}.$$

Obtained on the basis of effective potentials thermodynamic properties were used for solving the Hugoniot equation [3] which describes the relationship between thermodynamic properties on both sides of a shock wave. Impact of the non-isothermality on the Hugonio of dense plasma taking into account quantum diffraction effect is studied.

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ismagambetova@physics.kz

Liquid-liquid phase transition of dense hydrogen: Nuclear quantum and nonlocal exchange-correlation effects

Binbin Lu, Dongdong Kang*, Jiayu Dai

Department of Physics, College of Science, National University of Defense Technology, Changsha, Hunan 410073, P. R. China

The phase dynamics of dense hydrgoen is much interesting. Since now, first principles molecular dynamics is the most important method to study it in theory. Nuclear quantum effects and van der Waals interactions can be included, but many-body effects such as self-interactions and nonlocal exchange correlation effects are difficult to include because of extremely expensive computational costs. We study the liquid-liquid phase transition (LLPT) of dense hydrogen using first-principles molecular dynamics with hybrid functionals[1] with a accelerated scheme model. The efficient path integral method PI+GLE[2] is employed to consider the nuclear quantum effects, which play an important role in LLPT of dense hydrogen. The semi-empirical force-field correction (DFT-D3)[3] is used to account for van der Waals interactions between hydrogen molecules. By including nuclear quantum effects and van der Waals interactions in hybrid functional DFT calculations, the molecular dissociation is described more accurately than conventional DFT calculations[4]. We obtain the accurate temperature-pressure boundary of LLPT based on analysis of radial distribution function and vibrational spectra of hydrogen molecules, and the phase transition from molecuar phase to atomic phase is expected to change much.

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* email: ddkang@nudt.edu.cn

Energy deposition and implosion time in dense plasmas of heavy ion inertial confinement fusion

S.K. Kodanova*, T.S. Ramazanov, M.K. Issanova

Institute of Experimental and Theoretical Physics,
Al-Farabi Kazakh National University, Almaty, Kazakhstan

Investigation of interaction processes of ion beams with dense plasmas is one of the key problems in physics of inertial confinement fusion driven by heavy ion beams [1]. The stopping power is an important quantity used to describe the interaction of particle beams with matter. In the field of particle- driven inertial confinement fusion, interaction of highly charged ions with dense plasmas is of special interest [2-3].

Consequently, knowledge of dynamical characteristics of plasma ions in the ICF, such as the implosion time, energy deposition, penetration depth and the effective range in the plasma will enable us to calculate the design of thermonuclear target more accurately. These properties of plasma can be calculated accurately taking into account both quantum and collective effects in plasmas.

In this work energy losses in dense plasma are obtained on the basis of Coulomb logarithm using the effective potentials for ICF plasma [4-5]. These interaction potentials take into consideration long-range many-particle screening effects as well as short-range quantum-mechanical effects [6]. The values of energy deposition, energy partition, and implosion time in a wide range of densities and temperatures for inertial confinement fusion applications have been calculated. The obtained results for energy loss of particles and other energetic characteristics in dense plasma are compared with the available experimental data and theoretical results of other authors [7].

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* email: kodanova@physics.kz

Electrostatic and phonon properties of multicomponent Coulomb crystals

Kozhberov A. A.[*1]

[1] *Ioffe Institute, Saint Petersburg, Russia*

Matter in cores of old white dwarfs and in neutron star crusts consists of fully ionized ions arranged in a crystal lattice and neutralizing electron background. It is convenient to use the model of Coulomb crystal with uniform electron background for description of such systems. Among all Coulomb lattices which have ever been studied the body-centered cubic (bcc) lattice has the lowest electrostatic energy. However this statement is primarily related to one-component crystals (all ions are identical), while for multicomponent systems formation of other types of lattices is not excluded. In this work we consider electrostatic and phonon properties of various multicomponent Coulomb crystal lattices.

An analysis of the phonon spectra shows that binary bcc Coulomb crystal is stable if the ratio of ion charges (q) lies between 1/3.6 and 3.6, so that sufficiently different ions can't form the bcc lattice. On the other hand the binary magnesium diboride lattice is stable if q is greater than 0.1 but smaller than 0.375. A study of the binary hexagonal close-packed lattice shows that this lattice changes its size. The distance between its hexagonal layers decreases with the growth of $|q\text{-}1|$ while the binary bcc lattice stays cubic at any q.

Also for some lattices the linear mixing rule was checked. It turned out that it was useful only for the binary bcc lattice.

* email: kozhberov@gmail.com

Fluid description of dense quantum plasmas in RPA and beyond

Zhandos Moldabekov[*1,2], **Michael Bonitz**[1], **Tlekkabul Ramazanov**[2]

[1] *Institut für Theoretische Physik & Astrophysik, Christian-Albrechts-Universität, Kiel, Germany*
[2] *Institute of Experimental and Thepretical Physics, Al Farabi Kazakh National University, Almaty, Kazakhstan*

The theoretical description of quantum plasmas must incorporate the quantum mechanical effects of the electrons such as diffraction, spin statistics, and correlations appropriately on the relevant scales. First-principle approaches such as quantum kinetic theory or non-equilibrium Greens functions as well as Time Dependent Density Functional Theory require substantial computational efforts, and simulation of large numbers of electrons are not feasible yet. Therefore, the quantum hydro dynamic (QHD) model became popular as a simplified approach for quantum plasmas [1]. In previous works on QHD, the quantum non-locality effect (diffraction), was taken into account via the Bohm potential which is equivalent to the first order gradient correction [2] whereas spin statistics was included by replacing the classical pressure by the Fermi pressure [1]. In order to reach agreement with the result of the random phase approximation (RPA) for the plasmon dispersion, both the Fermi pressure and Bohm potential were empirically corrected by multiplying to a constant factor [1]. In this form, QHD model was used for investigation of the different phenomena such us ion shocks [3] , nonlinear ion-acoustic waves [4] etc. However, as it was shown in Refs. [2, 5, 6], often QHD is used outside the range of applicability and even with incorrect explicit expressions. In the present work, a consistent QHD model is developed on the basis of which previous results are revised. Further a fully non-local Bohm potential is derived on the basis of the RPA, which goes beyond of the gradient expansion approximation. Consideration of the non-ideality effects is based on the linking of the QHD exchange-correlation potential to dynamic local field corrections. As a result, the explicit form of the exchange-correlation potential in relaxation time approximation is given. Generalization of this approximation via introduction of the dynamic collision frequency as well as by making use of the method of moments are discussed. Finally, the range of applicability of QHD is analyzed.

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* email: zhandos@physics.kz

Melting line and DC conductivity of helium at high pressures

M. Preising[*1], **R. Redmer**[1]

[1] *University of Rostock, Rostock, Germany*

We studied the behavior of solid and fluid helium under high pressure with molecular dynamics simulations based on density functional theory (DFT-MD). Helium, as the second abundant element in nature, is important for astrophysical applications, e.g., the interior and evolution of gas giants and brown dwarfs. In particular, we calculated the melting line and examine the insulator-to-metal transition, both for extreme pressures up to the TPa region. The calculation of the melting line is a challenging topic in computational physics. Out of many approaches of different complexity and efficiency, two-phase simulations represent a very intuitive approach with high accuracy [1]. We have implemented this method and investigated finite-size effects and other convergence issues. We found good consistency with available experiments and gave predictions for the melting line of helium up to the TPa region.

Laser-driven compression experiments have shown that helium undergoes an insulator-to-metal transition with increasing density and temperature [2]. However, the exact location and nature of this transition is not clear yet. From the temperature and reflectivity measurements, the DC conductivity was inferred using a simple Drude model. We performed extensive DFT-MD simulations for the reported conditions and calculated the reflectivity and DC conductivity employing the Kubo-Greenwood formalism [3] and the PBE, vdW-DF1, and HSE exchange-correlation (XC) functionals. We found a significant impact of the XC functional on the DC conductivity, especially at lower densities and temperatures. We compared our results with available data [2,4].

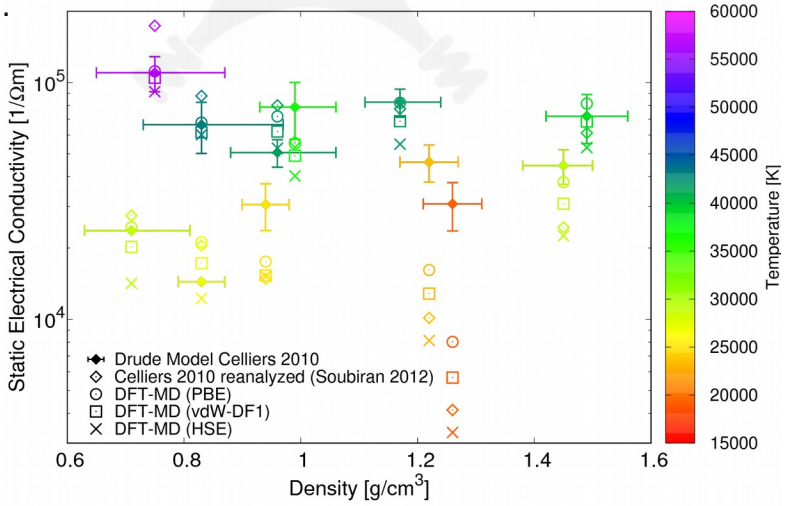

Figure: *Static electrical conductivity as reported by Celliers et al. [2] (filled diamonds), the revisited Celliers data by Soubiran et al. [4] (open diamonds), and our DFT-MD results (circles are PBE, squares are vdW-DF1, and crosses are HSE).*

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* email: martin.preising@uni-rostock.de

Directly calculated electrical conductivities of dense hydrogen from molecular dynamics

Qian Ma*, Jiayu Dai, Zengxiu Zhao

Department of Physics, College of Science, National University of Defense Technology, Changsha, Hunan 410073, P. R. China

The transport properties are important in warm and hot dense matter in which the Coulomb interaction is dominated in the scaterring process. The electronic quantum effects will play an important role on the transport properties since electrons are degenerated. Density functional theory (DFT) is considered as an effective method to investigate the transport proerties[1], but the dynamical collisions between particles are missed, and therefore will give larger quantities [2]. Here we use an electron force field (eFF) [3,4] method based molecular dynamics (MD) to include the electronic quantum effects to investigate the transport properties of wam dense hydrogen. The eFF method can be regarded as the development of wave packets molecular dynamics and it has been successfully used to decrible the thermodynamics of hydrogen, Auger process in diamondoids, the equation of states for dense lithium.The most important point of eFF method is assuming that each electron is considered as a Gaussian wave packet controlled by position and size while ions are still charged points. The electrical conductivity is calculated via the correlation of current. The results show that electronic quantum effects are important on the transport properties in warm dense hydrogen such as diffusion coefficient and electrical conductivity, which is much smaller than the results from DFT calculations.

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* email:maqian520@nudt.edu.cn

Comparison of path integral and quantum statistical approach for Stark broadening of Lyman lines in H-plasma

Heidi Reinholz[1], **Nacira Bedida**[*1, 2], **Gerd Röpke**[1]

[1] *Institute of Physics, University of Rostock, Rostock, Germany*
[2] *Institute of Physics, Unversity Kasdi Merbah-Ouargla, El Oued, Algeria*

New results for Lyman lines from hydrogen plasmas are presented using the path integral approach (PIA). The time evolution operator matrix elements in the dipole auto-correlation function are expressed by Feynman propagators. This involves summing up of perturbation series and applying the electric dipole selection rules to each term. Comparison with the quantum statistical approach (QSA) [1-4] for line profiles is performed in the temperature range $T = 10^4$ to 10^7 K and the electron density range $n_e = 10^{23}$ to 10^{26} m^{-3} assuming a quasi static ionic microfield as well as ion dynamics within the model microfield method (MMM) using Holtsmark [5] and Hooper [6] ion microfields. For electrons, PIA applies the electron collision operator given by Griem et al. [7]. For QSA, the electron impact collisions are treated in Born approximation, Born approximation supplemented with a cut-off and T-matrix approach. In general, good agreement is obtained, in particular, for low density and high temperature.

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* email: nacira.bedida@uni-rostock.de

Collision processes in partially ionized plasmas

Sebastian Rosmej[*1], **Heidi Reinholz**[1], **Gerd Röpke**[1]

[1] *Institute of Physics, University of Rostock, Rostock, Germany*

The conductivity of partially ionized plasmas is considered within the Linear Response Theory in a chemical picture. Correlation functions are evaluated including strong collisions via the T matrix approximation for different densities and temperatures. Beside electron-ion collisions [1] further scattering mechanisms (electron-electron and electron-atom) contribute to the electrical resistivity. Especially the influence of electron-electron collisions is important at high temperatures T>5 eV, see [2], and of electron-atom collisions for low temperatures T<5 eV, see [3]. For the electron-atom interaction in noble gases we suggest an optical potential [4] which reproduces the experimental observed Ramsauer minimum [5]. For application in plasma systems the optical potential is extended including screening effects.

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* email: sebastian.rosmej@uni-rostock.de

Free-free absorption coefficients in white dwarf atmosphere

N.M.Sakan*[1], V.A.Srećković[1], Z.Simić[2], M.S.Dimitrijević[2,3]

[1] University of Belgrade, Institute of Physics, P. O. Box 57, 11001, Serbia
[2] Astronomical Observatory, Volgina 7, 11060 Belgrade 74, Serbia
[3] Observatoire de Paris, 92195 Meudon Cedex, France

The contribution of free-free i.e. inverse bremsstrahlung to the total absorption in stellar atmospheres is not so important, but its contribution increases with density, and for very dense plasmas it becomes dominant. For example, authors [1] stated that inverse bremsstrahlung is the dominant absorption mechanism for lasers with parameters typical for inertial confinement fusion. Plasma in inertial confinement fusion experiments has properties which are similar to the conditions in stellar interiors. Consequently, it is of interest to investigate the role of inverse bremsstrahlung in deeper layers, and to examine its influence on radiative transfer through such layers.

In this contribution we present the free-free i.e. electron-ion inverse "Bremsstrahlung" characteristics for the case of the white dwarf atmospheres where such plasma characteristics as plasma density and temperature change in wide region. It is shown that determination of these characteristics such as the absorption coefficients and Gaunt factors can be successfully performed in the whole diapason of electron densities and temperatures which is relevant for the corresponding non-ideal, dense plasma of white dwarf atmospheres.

The Cut-off form of Coulomb potential is used to approximate the shielding effect in order to derive the absorption coefficients. The used quantum mechanical method of the calculation of the investigated characteristics is described and discussed in details in the papers of Mihajlov et al. [2,3]. The results are obtained for the DB White dwarf models (Koester 2015 private communication) in the wavelength region 100 nm < λ< 3000 nm. The range of the physical parameters covers the area important for plasma modeling from astrophysical standpoint (white dwarfs, central stars of planetary nebulae, etc). Also, these results can be of interest and use in investigation of different laboratory non-ideal, dense plasmas.

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* email: nsakan@ipb.ac.rs

HF electric properties of the astrophysical plasmas under extreme conditions

V.A.Srećković[1], N.M.Sakan[*1], Z.Simić[2], Lj.M. Ignjatović[1], M.S.Dimitrijević[2,3]

[1] University of Belgrade, Institute of Physics, P. O. Box 57, 11001, Serbia
[2] Astronomical Observatory, Volgina 7, 11060 Belgrade 74, Serbia
[3] Observatoire de Paris, 92195 Meudon Cedex, France

For further investigation of strongly correlated plasma physics, the investigations of its electronic properties remains an ongoing problem. For example theoretical calculations and measurements of reflectivity are important because of its possible use as diagnostic tool in the physics of high-density energy [1].
Here we determine the HF characteristics of astrophysical, dense, non-ideal plasmas on the basis of numerically calculated values for the dense plasma conductivity in an external HF electric field. The examined range of plasma frequencies covers the IR, visible and UV regions and consider electronic number density and temperature important for different stellar models.
These results, can be applied in the experiments of high pressure discharge, shock waves etc., where strongly non-ideal plasmas, including extremely dense plasmas, are created. Also the results presented here are important for investigation of atmosphere plasmas of astrophysical objects like white dwarfs with different atmospheric compositions (DA, DC etc.), and for investigation of some other stars (M-type red dwarfs, Sun etc.) as well as for laboratory plasma research (see e.g. [2,3]).

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[*] email: nsakan@ipb.ac.rs

Electrical conductivity of dense semiclassical plasma

K.N. Dzhumagulova (1), E.O. Shalenov (1), T.S. Ramazanov (1), H. Reinholz (2), G. Roepke (2)
(1) IETP, al-Farabi Kazakh National University, Al-Farabi 71, Almaty 050040, Kazakhstan
(2) Institute of Physics, University of Rostock, D-18051 Rostock, Germany

During the last few years many papers about the transport properties of dense plasmas have been published. The electrical conductivity in fully ionized hydrogen plasma is well investigated [1-3]. Besides hydrogen, noble gases are widely studied in plasma physics because of their simple electronic structure as closed shell systems. Especially, the electrical conductivity is of interest: Various experiments were performed measuring the electrical conductivity of helium [4, 5, 6], neon [4, 7], argon [4, 6, 7], krypton [4, 8], and xenon [4, 6, 7, 9].

In this paper we will consider fully ionized hydrogen plasma, that means with temperatures between lot 10^4 K and 10^7 and densities up to the pressure ionization limit. In the fully ionized plasma state the electrical conductivity is determined only by the scattering of free electrons (e) and protons (p). Therefore we have to take into account the formation, the decay and the scattering of bound states in two, particle collisions.

Based on the effective potential [10] the transport properties of the plasma particles were investigated. Quantum mechanical method of phase functions and Born approximation were used for their calculation. The results are compared with data of other theoretical and experimental.

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Phonons and heat capacity of magnetized Coulomb crystals of ion with polarizable electron background

Kozhberov A. A.[*1], **Baiko D. A.**[1]

[1] *Ioffe Institute, Saint Petersburg, Russia*

It is thought that the matter in cores of old white dwarfs and in neutron star crusts could be described by a model of Coulomb crystal: point-like ions arranged in a crystal lattice and neutralizing electron background. Usually electron background is considered to be uniform but for a more adequate description of such systems interactions between electons and ions have to be taken into account. In this work we present an analysis of phonons in Coulomb crystals with effects of electron screening and magnetization of the ion motion taken into account simultaneously. The heat capacity of such sustems is also calculated. It is shown that at low temperatures the heat capacity of Coulomb crystals in magnetic field could increase by several orders; at the same time the effect of polarization of the electron background does not exceed several tens of percent.

This work was supported by Russian Science Foundation grant 14-12-00316.

* email: kozhberov@gmail.com

Impact of the dipole-dipole interaction induced by an external field on the transport properties of dusty plasmas

A. Gabdulin[*1, 2], T. S. Ramazanov[1] , and Zh. A. Moldabekov [1]

[1] *Institute of Experimental and Theoretical Physics, Al Farabi Kazakh National University, Almaty, Kazakhstan*
71 Al-Farabi ave., 050040 Almaty, Kazakhstan and
[2] *Institute of Applied Sciences and Information Technologies,*
40-48 Shashkin str., 050038 Almaty, Kazakhstan

Study of the two-dimensional systems with the Yukawa interparticle interaction potential is of prime importance as such systems play a key role in plasma physics, physics of colloids as well as condensed matter physics [1–3]. In this report we present the study of sound speed, mean square displacement, and oscillations spectrum in the two-dimensional Yukawa liquids by molecular dynamics simulation where the interparticle interaction potential in addition to the Yukawa term has the dipole-dipole interaction term. The interaction potential obtained by multipole expansion of the screened Yukawa potential, which takes into account nonzero dipole moment of the particle, is used [4]. This procedure is similar to the well-known multipole expansion of the Coulomb potential. The dipole moments of particles are taken to be equal and parallel to each other. As a result, the contribution of the charge-dipole interaction to the total interparticle interaction potential is equal to zero. In dusty plasma such an interparticle interaction can arise as a result of creation of a compound particle (charged dust particle + focused ion cloud) due to ion streaming [5, 6] (for example, in the experiments where an additional external constant field is applied to the RF discharge [7]).

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* email: ayat_94@mail.ru

Exact calculation of the linear OCP response functions at strong coupling

Péter Magyar*[1], Zoltán Donkó[1,2], Gabor J. Kalman[2], and Kenneth I. Golden[3]
[1]*Institute for Solid State Physics and Optics, Wigner Research Centre for Physics, Hungarian Academy of Sciences, H-1121 Budapest, Konkoly-Thege Miklós Street 29-33, Hungary*
[2]*Department of Physics, Boston College, Chestnut Hill, Massachusetts 02467, USA*
[3]*Department of Mathematics and Statistics, and Department of Physics, University of Vermont, Burlington, Vermont USA*

We compute the frequency- and wave-number-dependent linear response functions of the three-dimensional Coulomb OCP in the strongly coupled liquid phase. The starting point of the calculations is the determination of the 2-point dynamical structure function via molecular dynamics simulation. In the consecutive steps we make use of the Fluctuation-Dissipation-Theorem and carry out numerically the Kramers-Kronig transform based on a Fourier series method. In these two steps we obtain the imaginary and the real parts of the external, longitudinal density response function, respectively. From these, we calculate the total density response and the dielectric response functions. The calculations are carried out for a set of different values of the coupling parameter. The imaginary part of the dielectric function provides important novel information about the damping of the collective modes. We demonstrate the expected [1] violation of the Kramers-Kronig relations for the dielectric function and we examine its dependence on coupling parameter and as a function of the frequency and wave-number domain.

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This work has been supported by the grant NKFIH 119357 and NSF.

*email: magyarpetery@gmail.com

OCP quadratic response functions

Péter Magyar*[1], Zoltán Donkó[1,2], Gabor J. Kalman[2], and Kenneth I. Golden[3]
[1]*Institute for Solid State Physics and Optics, Wigner Research Centre for Physics, Hungarian Academy of Sciences, H-1121 Budapest, Konkoly-Thege Miklós Street 29-33, Hungary*
[2]*Department of Physics, Boston College, Chestnut Hill, Massachusetts 02467, USA*
[3]*Department of Mathematics and Statistics, and Department of Physics, University of Vermont, Burlington, Vermont USA*

We present a method that allows us to compute the external (screened), quadratic dynamical density response function of the Coulomb OCP in the strongly coupled liquid phase. The method is based on perturbed molecular dynamics simulations, which allow the measurement of the space- and time-dependent density response of the system to an external, longitudinal dynamic perturbation. The Fourier analysis of the density profiles yields the linear and quadratic external response functions. The linear response function has also been computed from the 2-point dynamical structure function provided by unperturbed equilibrium MD simulation via the linear Fluctuation-Dissipation-Theorem and the Kramers-Kronig relation [1]. The good agreement of the linear response functions, obtained in the two different ways, validates our perturbative method. Combining then the linear dielectric function with the external (screened) quadratic response function we obtain the total (proper) dynamical quadratic response function for the OCP.

[1] Abstract „*Exact calculation of the linear OCP response functions at strong coupling*" at this Conference

This work has been supported by the grant NKFIH 119357 and NSF.

*email: magyarpetery@gmail.com

Dust chain formation and interaction with ion wakefield

L. S. Matthews[*1], B. Brooks[1], P. Hartmann[1,2], Z. Donkó[2], M. Rosenberg[3], and T. W. Hyde[1]
[1] Center for Astrophysics, Space Physics, and Engineering Research (CASPER), Baylor University, Waco, Texas, USA
[2] Wigner Research Centre for Physics, Budapest, Hungary
[3] University of California at San Diego

In many environments, positive ions in the plasma have a directed flow with respect to the negatively charged dust grains. The resulting interaction between the dust and flowing plasma creates an ion wakefield downstream from the dust particles, with the positive space region modifying the interaction between the charged grains and contributing to the observed dynamics and particle structure. Since the force exerted by the ion wakefield is weak, the effects are usually masked by gravity for terrestrial experiments. The PK-4 experiment on board the International Space Station allows experiments to be conducted in microgravity, and thus the underlying physics behind self-ordering of interacting complex plasma dust particles in field-aligned chains can be investigated.

Data obtained from orbit will be compared with data from two different ground-based experiments: a stratified and/or homogeneous DC glow discharge and a GEC RF reference cell with a glass box placed on the lower electrode, used to confine the particles in a vertical chain. Numerical modeling of both the plasma environment and dust dynamics will be used to predict the parameter space where particular wave modes in the dust structures can exist in experiment.

Here we report preliminary results of numerical models of the plasma discharge, wakefield and particle interactions in the three distinct environments. An *axisymmetric PIC/MCC* and *hybrid discharge simulation* is adapted to model the discharge conditions in the PK-4 and a ground-based DC glow discharge and determine grain equilibrium positions. The local plasma parameters are then used to calculate dust grain charges and the formation of the ion wakefield. Ultimately, charging and dynamics of the grains will be coupled self-consistently in an N-body code. Pair correlation functions obtained from the grain dynamics will enable exploration of dusty plasma phenomena in the strongly coupled liquid phase. The behavior of waves in the 1D electrorheological chains will be characterized as the coupling ranges from the crystal phase through the liquid phase

[*] email: lorin_matthews@baylor.edu

Chemical model of dusty plasmas

Mukhametkarimov Ye.S.[*1], **Kurbanov F.**[1], **Davletov A.E.**[1]

[1] *Al-Farabi Kazakh National University, Science Research Institute of Experimental and Theoretical Physics, Almaty, Kazakhstan*

Among modern researches in the field of plasma physics, a special attention is paid to the so-called dust or complex plasmas, which are originated at the contact of the plasma medium with the walls of experimental setups. This is prescribed to the fact that penetration of the solid state particles into the medium is responsible not only for a significant change in the local plasma characteristics, but also results in the interesting, from the fundamental point of view, collective behavior of the microparticles.

This report constitutes one of the first successful attempts [1] to construct a self-consistent theory of the thermodynamic properties of dusty plasmas at thermodynamic equilibrium, which must necessarily include the determination of the dust charge. In the model used herein, the dust particles are considered as hard balls, which are actally potential wells for electrons and are characterized by some work function, such that it turns principally possible to describe not only the electron absorption, but the electron emission as well.

It is assumed that the plasma medium itself consists of four types of particles, i.e. electrons, ions, neutral atoms and dust particles that can absorb or emit electrons. Based on the solution of the generalized Boltzmann-Poisson equation [2], the free energy of the four-component system of interest is constructed and its further minimization allows one to determine both the ionization degree of the plasma and to obtain the electric charge of the dust particles. This opens up a new ground for studying the effect of dust particles on the ionization equilibrium in a plasma.

The proposed approach provides a self-consistent scheme to evaluate the correlation functions and thermodynamic characteristics of the entire dusty plasma, rather than its individual components.

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* email: ye.mukhametkarimov@gmail.com

Cage correlation functions of dust particles in a background gas and external magnetic field

Masheyeva R.U. [1], **Dzhumagulova K. N.** [*1] , **Ramazanov T.S.** [1], **Donkó Z.**[2], **Xia G.**[3]

[1] *IETP, al Farabi, Kazakh National University, 71, al Farabi av., Almaty, 050040, Kazakhstan,*
[2] *Institute for Solid State Physics and Optics, Wigner Research Centre for Physics, Hungarian Academy of Sciences, Budapest, Hungary*
[3] *The University of Manchester, Manchester, UK*

In this work we investigate the influence of a static homogeneous external magnetic field and background gas medium on the quasi-localization of the particles - characterized quantitatively by cage correlation functions [1] - in strongly coupled two-dimensional Yukawa systems. We use the Langevin dynamics computer simulation method. The equations of motion of the particles are written as:

$$m\ddot{\vec{r}}_i = \sum_{i \neq j} \vec{F}_{ij}(t) + Q\dot{\vec{r}}_i \times \vec{B} - vm\dot{\vec{r}}_i + \vec{\zeta}_i(t) \quad , \qquad (1)$$

where the first term on the right hand side gives the sum of inter-particle interaction forces, the second is the Lorentz force, the third term that represents the friction force (proportional to the particle velocity), is due to of the presence of the background gaseous environment, while the fourth term accounts for a randomly fluctuating “Brownian” force that is caused by the random kicks of the gas atoms on the dust particles. To integrate the equations of motion (1), a new numerical scheme is used, in which the time step does not depend on the magnitude of the magnetic field [2]. This scheme was obtained similarly to the scheme proposed in Ref. [3], but takes into account the friction force. The results are consistent with those obtained in [1, 4] in the limiting cases, when the frictional force (and random force) or the Lorentz force is equal to zero, respectively.

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* email: ranna_m@mail.ru

Calculating structural characteristics of one-component plasmas

Kh. Santybayev*[1], Yu.V. Arkhipov[1], A. Askaruly[1], A.E. Davletov[1], D.Yu. Dubovtsev[1], I.M. Tkachenko[2]

[1] Al-Farabi Kazakh National University, Almaty, Kazakhstan
[2] Universidad Politécnica de Valencia, Valencia, Spain

Practical application of research results on one-component plasma has found its reflection in various areas, such as astrophysics, lithography, dusty plasmas, ultracold plasmas, etc. Therefore, study of static and dynamic properties of OCP is of significant importance.

There is a number of theoretical methods of calculation of the static characteristics based on integral equations, fitting approximations and empirical formulas with the results of simulations often taken as reference. In this case, it is traditionally accepted that the theoretical results should be in a good agreement with the latter.

Not all of the above theoretical methods can be employed to calculate dynamic characteristics by the method of moments [1]. In the present work, we propose to qualify the static characteristics through the Hölder or Cauchy-Schwarz inequalities for the application of the above methods, $b>0$. The function b depends on the plasma thermodynamic characteristics via the static structure factor.

Precisely, we consider the hyper-netted chain (HNC) approximation with and without the empirical bridge function proposed by Ng [2], the modified HNC approximation (MHNC) [3], the variational modified HNC (VMHNC) [4], and other empirical and fitting formulas, e.g., [5]. For example, in Figure we present data for the HNC and the VMHNC, and show that in one case the inequality is violated.

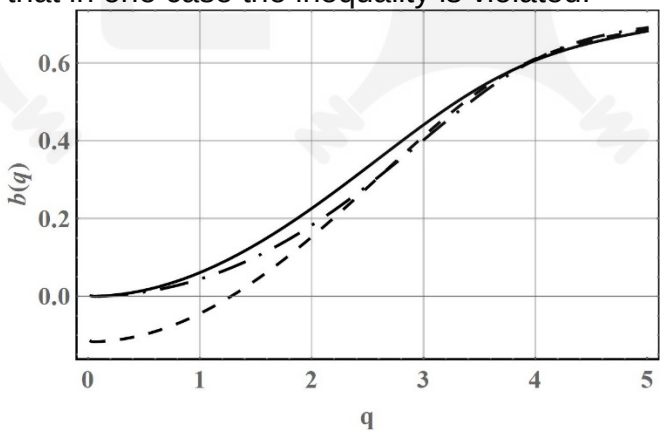

Figure: *Criterion of satisfaction of the Cauchy-Schwarz inequality, b>0, at Γ=16 for various theoretical methods: HNC (solid line); HNC with the bridge function [2] (dashed line); VMHNC [4] (dot dashed line).*

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* email: kh.santybay@googlemail.com

Classical Dynamics of Asymmetric Charged Particle Bilayers

Luciano Silvestri[1]*, Gabor J. Kalman[1], Zoltan Donko[1,2], Peter Hartmann[1,2], Kenneth I. Golden[3]

[1] *Department of Physics, Boston College, Chestnut Hill, Massachusetts, 02467, USA*

[2] *Institute for Solid State Physics, Wigner Research Centre for Physics, Hungarian Academy of Sciences, Budapest, Hungary*

[3]*Department of Mathematics & Statistics & Dept. of Physics, University of Vermont, Burlington, VT 05405, USA*

Recently, the existence of Fano-like anti-resonances (FLA) in the partial dynamic structure factor of strongly coupled binary ionic mixtures [1] was demonstrated. A theoretical model, based on the Quasi Localized Charge Approximation (QLCA), has shown that these FLA-s are governed by the microscopic drag between the current fluctuations of the two species. Charged particle (electron-electron or electron-hole) bilayers are parallel planes occupied by interacting particles and separated by a distance comparable to the inter-particle distance within the layers. These systems can be viewed as a binary system, where the two species are distinguished from each other not by different parameters, but by the difference between the intralayer and interlayer potentials. Therefore, it is expected that FLA-s exist in these systems as well. In this study, we apply the extended-QLCA (ex-QLCA) [1] to bilayers and show that this is indeed the case, but only when the symmetry between the layers is broken (e.g. different masses or densities), while no FLA-s are present in the symmetric case. In this study, we concentrate on the e-e bilayer. We have performed detailed Molecular Dynamics (MD) computer simulations on the system, for a wide range of coupling parameter, $\Gamma = \{1 - 120\}$ values, which confirm the results of the theoretical analysis.

With the new results derived from the MD simulations we have also extended previous work on the collective spectrum of symmetric and asymmetric bilayers [2-3]. Both theory and simulations show that in the asymmetric case the collective spectrum of the strongly coupled regime consists of a longitudinal quasi-acoustic in-phase and a gapped out-of-phase mode. While the existence of the gapped mode is predicted by the QLCA (in contrast to the RPA), there is a discrepancy between the predicted value and the one obtained by the MD simulation. The mode appears around $\Gamma = 5$ and its value at $k = 0$ does not seem to change at higher coupling values. At weak coupling, the RPA predicts the existence of an out-of-phase acoustic mode. The simulation results do not show the presence of such a mode in the moderately coupled $1 < \Gamma < 5$ regime, even in the absence of the gapped excitation. The effect of the asymmetry appears in the lowest order (in k) correlation-independent contribution to the quasi-acoustic mode; in the strong coupling regime, the oscillation frequency is governed by the heavier species, while in the weak coupling regime it is the lighter species that is dominant, as predicted by the QLCA [3]. This research is supported by the NSF and by NKFIH-119357

Electrical probe diagnostics of asymmetric RF discharge plasma with confined nanodust particles

Y.A. Ussenov*[1], E. von Wahl [2], T.S. Ramazanov[1], H. Kersten[2]

[1] NNLOT, IETP, KazNU, Al-Farabi av. 71, 050040, Almaty, Kazakhstan
[2] IEAP, University of Kiel, Leibnizstr. 11-19, 24098 Kiel, Germany

Basic principles of nanoparticle synthesis technology in plasma of gas discharges are determined by physical and chemical processes occurring in the "dusty" or "complex" plasma. During the cyclic particle growth process nanoparticles confined in a plasma volume of gas discharge due to the influence of Coulomb, neutral drag and gravitational forces and changes the plasma parameters [1]. Using the universal plasma diagnostics method such as the Langmuir probe, which is quite successfully used in dusty plasmas of inert gases with micron particles [2], causes some difficulties in its application in the chemically active gas discharge plasma containing nanoparticles. The main difficulty is contamination of the probe surface and deposition of thin dielectric films on the probe tip. This leads to the distortion of the I-V curve of the probe and incorrect interpretation of the data.

This work presents the results of probe measurements of temperature, electron density, and plasma potential in an argon - acetylene plasma in an asymmetric RF discharge (13.56 MHz) with nanoparticles [1]. The problem with the probe surface contamination by charged nanoparticles was solved by application of a sufficiently fast "complex" sweep of the probe voltage and a combination of ion bombardment and electron heating. The results were obtained at different phases of nanoparticle growth and compared with the voltage measurements of the discharge self-bias. It was shown that the electron concentration decreases due to the surface absorption by nanoparticles during charging, whereas the electron temperature and plasma potential increase. The data on the influence of nanoparticles on the plasma parameters obtained by the probe method and the applied method itself maybe used in further detailed studying of the processes of nanoparticle synthesis in low-temperature plasmas.

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*email: yerbolat@physics.kz

Obtaining of carbon nanoparticles in combined RF/DC discharge plasma

A.T. Zhunisbekov [1], T.S. Ramazanov[1], S.A. Orazbayev[1,2], M.K. Dosbolayev[1,2], M.T. Gabdullin[2], D.B. Omirbekov[2]

[1] Institute of Experimental and Theoretical Physics, Al-Farabi Kazakh National University, Almaty, Kazakhstan
[2]National Nanotechnology Laboratory of the Open Type, Al-Farabi Kazakh National University,Almaty, Kazakhstan,

Nowadays nanoparticles and nanostructured materials are used widely in human activities. Production of such materials in plasma medium has some advantages. Combined discharge (RF/DC) is used for etching various materials, for sterilization, plasma cleaning etc.. Papers [1-3] contain experimental and analytical results of ignition of lengthwise combined RF/DC discharge in argon and nitrogen. In addition, combined discharge is studied for particle manipulation in plasma medium. Authors of [4] have synthetized tungsten nanoparticles in DC plasma. The dependencies of particle sizes on parameters of RF capacitive discharge plasma was obtained in [5]. In present work we used the combined RF/DC discharge plasma for synthesis carbon nanoparticles.

Experimental setup consists of several parts: power unit (RF generator with matching device and DC power unit), vacuum system and chamber. The main part of experimental setup is the system of electrodes, which is inside of chamber. Plasma is igniting between two round parallel electrodes of 10 cm in diameter. Interval between electrodes is 3 cm. The upper electrode connected to RF generator and DC power unit, lower electrode is grounded. Aim of graphite attached to upper electrode. RF discharge parameters vary in following ranges: power – 1-50W, DC voltage – 0-200V, gas pressure – 0.1-2 mbar.

As a result, distribution of particle sizes in accordance with plasma parameters, as well SEM image of samples has been obtained. SEM images show synthesized spherical nanoparticles with diameters from 80 to 500 nm in dependence on plasma parameters. The dependence of self-bias voltage on time at different plasma parameters (gas pressure and discharge power) has been obtained. The graph of dependence of particle synthesis time on DC voltage was shown. It was determined that as the DC voltage increases, the particle synthesis time decreases. Thus it can be concluded, that DC voltage can control growth of particles in plasma medium.

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The Uniform Electron Gas at Warm Dense Matter Conditions

Simon Groth,[1,*] Tobias Dornheim,[1] Travis Sjostrom,[2] and Michael Bonitz[1]

[1]*Kiel Univ., Germany*
[2]*Los Alamos National Lab., USA*

The availability of an accurate parametrization of the exchange correlation energy of the uniform electron gas (UEG) on the basis of ground state quantum Monte Carlo simulations has been crucial for the success of density functional theory (DFT) calculations within the local density approximation. However, it is widely agreed [1] that the description of recent experiments with inertial confinement fusion and laser-excited solids within the DFT framework requires to go beyond the ground state. While an explicitely thermodynamic DFT approach is long known, it requires an accurate parametrization of the exchange correlation free energy of the UEG at warm dense matter conditions. Here we present our novel parametrization [2] that is based on our recent ab initio simulations [3,4] and compare to various other parametrizations, including the recent parametrization by Karasiev et al. [5].

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*E-mail address: groth@theo-physik.uni-kiel.de

Simulation of dynamical properties of Hydrogen plasma by DFT-WPMD method

Yaroslav Lavrinenko[1], **Ilya Valuev**[*1],

[1] *Joint Institute for High Temperatures of RAS, Moscow, Russia*

A combination of Density Functional and Wave Packet Molecular Dynamics methods is proposed to simulate the thermodynamics and the electronic dynamical properties of the nonideal plasma. In this approach we use the non-antisymmetrized single-Gaussian wave packets to represent electrons and point-like particles for ions. The kinetic and electrostatic energy contributions for electrons are calculated within the WPMD model, whereas the exchange-correlation energy and its derivatives with respect to the dynamic variables is evaluated on a space mesh. Although more computationally demanding than the original WPMD method, the proposed technique allows one to account for both exchange and correlation effects within the dynamical electron model. The use of GPU acceleration for computing the exchange-correlation energy contribution is very effective and compensates the extra computational costs.

In this work we benchmark the DFT-WPMD using the basic LDA exchange-correlation functional with the simple models (homogenous electron gas, atomic and molecular hydrogen) and with the hydrogen plasma equation of state. We show, that unlike the non-antisymmetrized WPMD model, the new technique predicts qualitatively correct bound states for the atomic and molecular hydrogen and does not suffer from the effects of the degenerate norm matrix, which slow down the antisymmetrized WPMD computation. All calculations are performed for a confined model which does not allow electron wave packets to spread infinitely.

We calculate the equation of state (internal energy and pressure) and the dynamical structure factors for hydrogen plasma for a range of densities from n_e=10^{21} to 10^{24} cm^{-3} and a range of temperatures form 10^3 to 10^5 K. The results for hydrogen plasma are compared with the predictions of the antisymmetrized WPMD, accounting for the exchange effects only and with other simulations including PIMC and DFT. The range of applicability, accuracy and performance of the new technique are discussed.

* email: valuev@ihed.ras.ru

Computer simulation of dynamic properties of dense plasmas using the theory of effective potentials

S.K. Kodanova*, T.S. Ramazanov, M.K. Issanova

Institute of Experimental and Theoretical Physics,
Al-Farabi Kazakh National University, Almaty, Kazakhstan

At the present time the study of the dense inertial confinement plasma (ICF) properties is not only of fundamental interest, but it also has various important technological applications [1]. To construct plasma systems it is necessary to take into account complicated processes in dense plasma. In this connection the role of computer simulations equipped with visualization methods for analysis of processes in dense ICF plasma is increasingly important.

Programs for simulation and calculation of inertial confinement fusion targets are very complicated and require a lot of computation time. The complexity of calculations is caused by the necessity of taking into account a large number of different physical processes simultaneously: transport of particles; plasma thermodynamics; energy absorption; radiation transport; stopping power, etc. Each part of the program related to the description of one or more of these processes is already rather complicated.

Progress in the theory of effective interaction potentials allows us to calculate the Coulomb logarithm, dynamic properties of weakly coupled as well as nonideal plasmas taking into account both collective screening and quantum diffraction effects. As a result, it is possible to calculate the above-mentioned properties of classical and semiclassical plasmas without using time-consuming simulation methods such as molecular dynamics simulation. For this purpose, user-friendly software with a wide range of functions for simulation of dynamic properties of dense plasmas using the theory of effective potentials is needed [2-4]. The range of applicability of the theory of effective interaction potentials is discussed and part of the software for simulation of the Coulomb logarithm and dynamic properties of dense plasmas is presented.

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* email: kodanova@physics.kz

Applicability of different atomistic simulation methods for calculation of thermodynamic properties of nonideal plasmas

Ya. S. Lavrinenko[*1,2], I. V. Morozov[1,2], I. A. Valuev[1]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia

In this work we report on evaluation of different simulations methods for studying electron–ion non-ideal plasmas or warm dense matter. As a test system we consider the hydrogen plasma in the temperature range of $T = 2 \times 10^4$–5×10^5 K and the non-ideality parameter values $\Gamma = 0.01$–6.

The internal energy and pressure are calculated using the classical molecular dynamics (MD), the wave packet molecular dynamics (WPMD) and wave packet Monte-Carlo (WPMC) [1-4]. Constraining boundary conditions with a harmonic wall potential are used for wave packets to prevent wavepacket spreading [5]. The self-consistency of this approach is discussed.

The second result is concerned with determination of the area of applicability of the classical MD within the above mentioned parameter range. For this, we compare the equation of state obtained by MD with the abinitio methods such as Path Integral Monte Carlo (PIMC) [6] and Density functional theory (DFT) simulations. We show that at certain plasma parameters the MD method fails due to appearance of unphysical ordered structures of particles. This turns out to be the effect of the non-Coulombic pseudopotential (both in electron-electron and ion-electron interactions).

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* email: lavrinenko@phystech.edu

Screening of ion potential in quantum non-ideal dense plasmas

Zh. Moldabekov[*1, 2], T. Dornheim[1], S. Groth[1], P. Ludwig[1], M. Bonitz[1], and T. S. Ramazanov[2]

[1] Institut für Theoretische Physik & Astrophysik, Christian-Albrechts-Universität, Kiel, Germany
[2] Institute of Experimental and Thepretical Physics, Al Farabi Kazakh National University, Almaty, Kazakhstan

Despite recent advances in modeling and computer simulations, a fully self-consistent treatment of highly nonequilibrium electron-ion plasmas has not been possible so far due to the requirement of the simultaneous account of electronic quantum and spin effects together with the (possibly) strong ionic correlations. The main problem here are the vastly different time scales of electrons and ions resulting from their different masses. A possible solution of this dilemma is a multi-scale approach that has been proposed by Ludwig et al. [1]. It takes advantage of the weak electron-ion coupling that allows for a linear response treatment of the electrons. The key of this multiscale approach is to absorb the fast electron kinetics into an effective screened potential of the heavy ions where the screening is provided by the electrons via a proper dielectric function. Recently, we have performed the analysis of the screened ion potential in the random phase approximation (RPA) [2]. The RPA result for screening in quantum plasmas is valid if the coupling parameter is less than unity. In this work we extend our analysis to the case of non-ideal quantum electrons by making use of local field corrections which are determined on the basis of the Quantum Monte Carlo data [3-5]. Analytical results obtained in the long wavelength limit are also presented. Particularly, obtained results are relevant to the non-ideal partially degenerate plasma of a neutron star atmosphere [6].

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* email: zhandos@physics.kz

Configuration Path-Integral Monte Carlo: localized and non-orthogonal basis

Xiaolei Zan[1], Jianmin Yuan[1]

[1] *Department of Physics, National University of Defense Technology, Changsha ,PR of China*

In the past few years, interest in the study of warm dense matter has grown increasingly. Path-Integral Monte Carlo (PIMC) is an important method to study this problem. The combination of Restricted PIMC [1](RPIMC) , Permutation Blocking-PIMC [2](PB-PIMC) , Configuration PIMC [3](CPIMC) and the Density Matrix QMC [4](DMQMC) makes it possible to overcome the Fermion Sign Problem (FSP) and finally figure out accurate results for a many-fermion system over almost the entire warm dense regime.

With the increase of the Wigner-Seitz radius rs, the UEG will eventually form the Wigner Crystal, the electrons become more and more localized, CPIMC is no longer applicable, while RPIMC is more suitable for calculation. We analyze that with the enhancement of the localization, the plane wave used by CPIMC is no longer suitable to describe the current system. If we employ the localized wave function (such as Gauss function), we will improve the average sign in CPIMC simulation.

We introduced the localized and non-orthogonal basis and proposed the corresponding modification in the calculation of the Hamiltonian matrix. By doing this, we intend to bridge the PIMC and CPIMC, since the limit of the Gauss function is delta function and the CPIMC in delta basis functions is similar to PIMC. We have successfully observed the phenomenon of electron localization, but the total energy is dependent to the localization parameter, a further research is to be undergoing.

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Pauli blocking by effective pair pseudopotential in degenerate Fermi systems of particles.

Larkin A.S.[1,2], **Filinov V.S.**[1]

[1] *Joint Institute for High Temperatures RAS, Moscow, Russia*
[2] *Moscow Institute of Physics and Tecnology, Dolgoprudny, Russia*

The main difficulty for path integral Monte Carlo studies of Fermi systems results from the requirement of antisymmetrization of the density matrix and is known in literature as the 'sign problem'. To overcome this issue the new numerical version of the Wigner approach to quantum mechanics for treatment thermodynamic properties of degenerate systems of fermions has been developed. The new path integral representation of quantum Wigner function in the phase space has been obtained for canonical ensemble [1]. Explicit analytical expression of the Wigner function accounting for Fermi statistical effects by effective pair pseudopotential has been proposed. Derived pseudopotential depends on coordinates, momenta and degeneracy parameter of fermions and takes into account Pauli blocking of fermions in phase space. The new quantum Monte-Carlo method for calculations of average values of arbitrary quantum operators has been proposed. To test the developed approach calculations of the momentum distribution function of the degenerate ideal system of Fermi particles has been carried out in a good agreement with analytical Fermi distributions. Generalization of this approach for studies influence of interparticle interaction on momentum distribution functions of strongly coupled Fermi system is in progress.

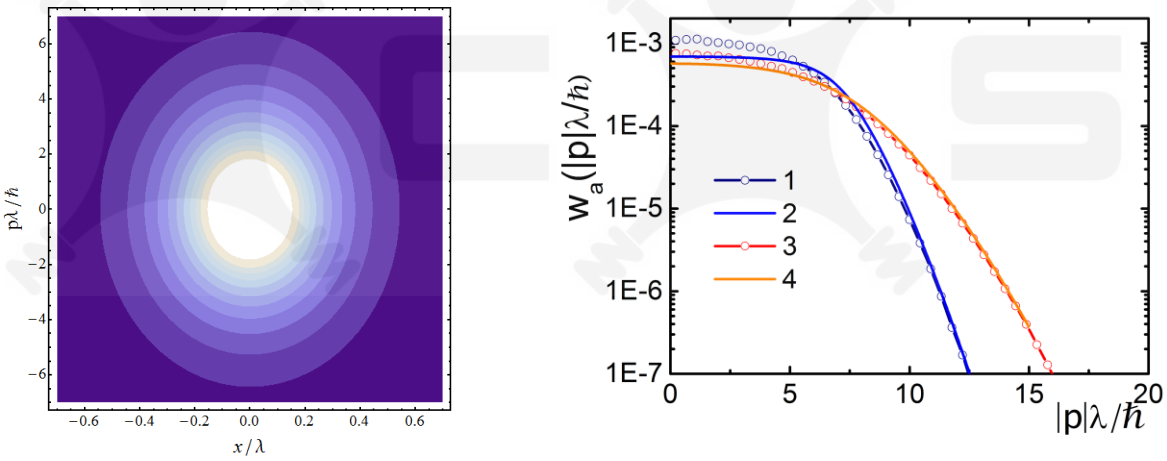

Figure: Left panel*: contour plots of the repulsive effective exchange pair pseudopotentials in phase space.*
Right panel*: The momentum distribution functions for ideal electron---hole plasma. . Lines:PIMC calculations - 1,3 ; Fermi distributions for electrons and two times heavier holes - 2,4. Parameter of degeneracy for electron is equal to 6.*

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* email: vladimir_filinov@mail.ru

X-RAY INVESTIGATIONS OF A HIGH – ENERGY-DENSITY PLASMA

George A. Pavlov*
Institute of Problems of Chemical Physics RAS, 142432 Chernogolovka, Moscow Region, Russia,
Valery M. Treushnikov and Victor V. Treushnikov
PC "Reper-NN",
Nizhny Novgorod, 603003, Russia

Any assumptions about plasma parameters require experimental evidence, especially in experiments with short laser pulses and beams of heavy ions. The use of optical methods in a visible range for studying "relief" of plasma is often impossible because of strong thermal environment irradiation, which must be blocked. Therefore, it is proposed to diagnose laser plasma in hard X-ray spectrum using polymer X-ray refractive lenses with axial symmetry [1], assembled into the compound lens with the required characteristics [2]. In our opinion, it is for the first time when the compound X-ray lens is used to investigate in hard x-rays the images of dense plasma generated under irradiation of copper foil by high-power laser pulse.

For realization of parameters, providing the necessary quality in manufacturing of shape memory polymer lens, a single-stage frontal photo-polymerization method was applied. The proposed imprinting method allows simultaneously to perform polymer photo-synthesis from photo-polymerization compositions and to produce polymer product of a given form with high accuracy. The assembly for lens manufacturing consists of quartz capillary and precision brass mold in the shape of paraboloid with rotational symmetry. Parabolic 3D refractive lenses from shape memory polymers were manufactured and tested using monochromatic X-rays of 10keV: efficiency and gain were measured and the radiation stability was performed.

Pilot scheme for the study of laser plasma under extreme condition is implemented using a compound 3D X-ray lens [2]. Hard X-ray image of laser plasma produced by irradiating of copper foil by intense laser pulse was recorded using this lens.
The image obtained with this lens, look more contrast, than image obtained by the pinhole camera, in principle, in much broader spectral range. It was shown that the use of compound X-ray lenses of the proposed design allows us to get local and detailed experimental data on spatial configuration (or temporal dynamics, if instrumentation is available) of laser plasma under extreme conditions, since its examination by optical methods is insufficient and difficult. The data on plasma sizes, degree of homogeneity, and dynamics become more reliable. These data can be correctly compared with computer simulation results of the relevant gas-dynamic processes implemented in full-scale experiments.

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*) *e-mail: pavl4411@yandex.ru*

K-alpha Emission Profiles of Warm Dense Argon Plasmas

Heidi Reinholz[1], **Andrea Sengebusch**[*1], **Gerd Röpke**[1]

[1] *Institute of Physics, University of Rostock, Rostock, Germany*

K-line profiles emitted from a warm dense plasma environment are used for diagnostics of Ar droplet plasmas created by high energy laser pulses. We observe temperature gradients within the Ar droplet from cold temperatures of the order of some 10 eV up to higher temperatures of over 200 eV. To describe the undisturbed emitters we consider ions up to Ar^{16+} in 111 different electronic configurations. Our aim is to take into account as much as possible of the atomic structure and to avoid averaging over configurations or using some kind of super-configurational approach. Hence, we use over 700 different ionization energy levels and over 1200 K-alpha emision lines, as tabulated in [1], to perform calculations of plasma effects and spectral line shapes. The plasma screening is considered within a perturbative approach to the Hamiltonian. This screening influences the many-particle system resulting in energy shifts due to electron-ion and electron-electron interactions. With this approach we get a good reproduction of the different features of experimental spectra obtained in spacially and temporally integrated measurements [2]. It becomes obvious, that spectral line shapes of inner shell transitions are strongly influenced by ionization and excitation processes within the plasma environment.
Comparing with the widely known FLYCHK code, detailed accounting for internal structure and treating plasma effects within our quantum statistical approach leads to a more detailed LTE temperature-density-relation (equation of state) as well as new results for the inferred temperature distribution from the experimental data [2].

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* email:andrea.sengebusch@uni-rostock.de

Simulation Studies of the Full Impact of Future Circular Collider Ultra-Relativistic Proton Beam on a Solid Copper Target

N.A. Tahir*[1], F. Burkart[2], R. Schmidt[2], A.Shutov[3], D. Wollmann[2] and A.R. Piriz[4]

[1]GSI Darmstadt, Germany
[2]CERN-AB, Geneva 23, Switzerland
[3]IPCP Chernogolovka, Russia
[4]University of Castilla-La Mancha, Ciudad Real, Spain

E-mail;**n.tahir@gsi.de**

Abstract: Beam-matter heating is an important problem relevant to every powerful accelerator for a number of reasons. For example, intense particle beams are considered to be an efficient tool to generate samples of High Energy Density (HED) matter in dedicated beam-target experiments [1,2]. Moreover, such studies are necessary for assessing the damage caused by the beam to the equipment and the accelerator components in case of an accident. In this contribution, we deal with the second aspect of the problem in case of the proton version of the Future Circular Collider (FCC-hh). Currently, an extensive design study is being done by the international scientific community to assess the feasibility of this, much more powerful post Large Hadron Collider machine. According to the optimum design parameters, the FCC will accelerate two counter rotating proton beams with particle energy of 50 TeV, in a circular tunnel with a circumference of 100 km. Each beam is comprised of 10600 bunches, with bunch intensity of 10^{11} protons. Bunch length is considered to be 0.5 ns while two neighboring bunches are separated by a gap of 25 ns. The transverse intensity distribution is Gaussian with a typical $\sigma = 0.2$ mm.

The total energy in each beam is about 8.5 GJ, which is equivalent to the kinetic energy of an Airbus A380 (560 t) flying at a speed of 850 km/s. To assess the consequences of an accident involving such a powerful beam, we carried out numerical simulations of the full impact of one FCC beam with a solid copper cylindrical target having a length = 5 m and a radius = 2 cm. The target is facially irradiated in a way that the target and the beam axis coincide. These simulations have been carried out using an energy deposition code FLUKA [3] and a 2D hydrodynamic code, BIG2 [4], iteratively. This study has shown that the static range of a single FCC proton in solid Cu is about 1.5 m, but the penetration length of the entire beam comprising of 10600 proton bunches becomes about 350 m due to the hydrodynamic tunneling. This has important implications on the machine protection design. Moreover, a big part of the target is converted into HED matter [5].

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Dielectric response function for warm dense matter states

Kushal Ramakrishna[1], **Jan Vorberger**[1]
[1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

The dynamic structure factor (DSF) is an important parameter to determine warm dense matter properties and can be accessed using x-ray Thomson scattering from energetic x-ray sources at LCLS, SACLA or EU-XFEL[1,2]. To improve upon the existing DSF models with greater accuracy and better description to model high pressure solids and liquids, a good agreement between theory and experiment is needed taking into account the electron-hole interaction resulting from an optical absorption, especially if the system is a semiconductor or an insulator. In a theoretical framework, we need access to the dielectric response function calculated using methods such as RPA, GW or even BSE based on density functional theory[3,4]. Small-gap semiconductors and metals, instead, screen this electron-hole interaction, and the resulting contribution can therefore be negligible. The Bethe-Salpeter equation indeed couples the electron and the hole, and has been very successful for the calculation of absorption spectra of a large variety of systems: insulators, semiconductors, atoms, clusters. We would like to present the results using aforementioned methods for different systems modelling warm dense matter states.

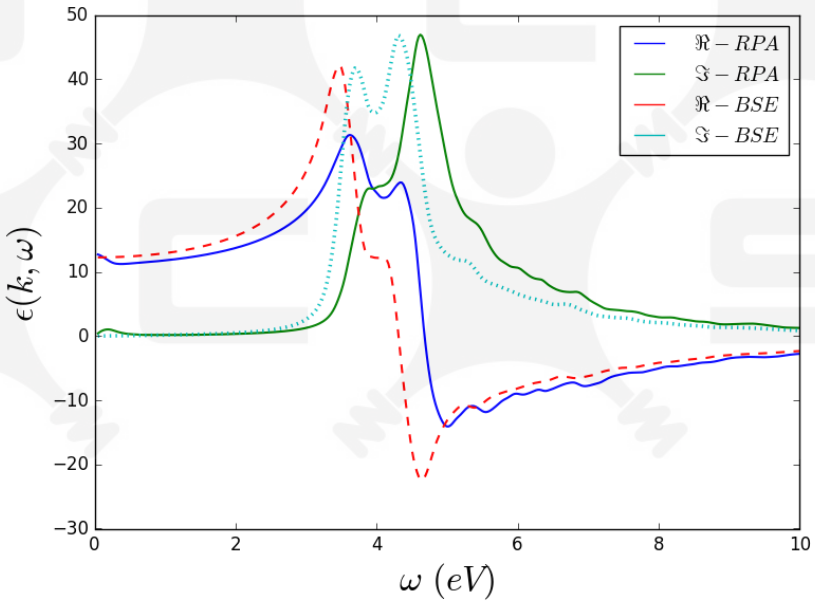

Figure 1: Dielectric function for Silicon

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[1]email:k.ramakrishna@hzdr.de

Generation of Planetary Interior Conditions in the Laboratory Using Intense Heavy Ion Beams at FAIR

N.A. Tahir*[1], I.V. Lomonosov[2], A.R. Piriz[3], B. Borm[1], A. Shutov[2], P. Neumayer[1], V. Bagnoud[1] and S. A. Piriz[3]

[1]GSI Darmstadt, Germany
[2]IPCP Chernogolovka, Russia
[3]University of Castilla-La Mancha, 13071 Ciudad Real, Spain

*E-mail;**n.tahir@gsi.de**

Abstract: The field of planetary physics has received a great boost due to the recent discoveries of extrasolar planets. Majority of these planets are believed to be gas giants like Jupiter, nevertheless a few Earth-like rocky planets named, super-Earths, have also been found. Due to the vast seismic data collected over the past many decades, the geologists have a reasonable idea about the structure of the Earth core. It is believed that the Earth core is mostly comprised of Fe. Assuming an Earth-like internal structure, models have been developed to assess the physical conditions that may exist at the interior of the super-Earths of different masses. It has been shown that [1,2] for planet mass between 1 – 10 times Earth mass, the pressure could be in the range of 3.5 – 15 Mbar while the temperature may be in the range 6000 – 10000 K. It is thus important to understand the thermophysical and transport properties of Fe under these extreme conditions in order to study the planetary interiors.

In this talk we present two-dimensional hydrodynamic simulations which show that using intense heavy ion beams that are going to be available at the FAIR accelerator in Darmstadt, one can perform experiments to generate High Energy Density (HED) samples of Fe with the above physical conditions. These samples can be used to study the equation of state properties, thermal and electrical transport properties as well as the viscosity of HED Fe. This study exploits the proposed LAPLAS (Laboratory Planetary Sciences) scheme [3,4], which is based on a low-entropy compression of a sample material driven by an intense ion beam in a multi-layered cylindrical target. Intense laser-driven hard x ray (100's of keV) will be used as a backlighter to enable imaging along the cylinder axis. This will provide a monitor of the hydrodynamic evolution of the target and will allow for absolute measurements of the final areal density reached in the sample.

Previously, simulations of this scheme were done to produce HED samples of hydrogen [3] and water [4] to generate the extreme physical conditions that exist in the cores of hydrogen rich planets like Jupiter and Saturn as well as water rich planets like Uranus and Neptune, respectively. We expect that these experiments will be very helpful in understanding the structures of the different type of planets in our solar system and elsewhere.

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The effect of dust particle polarization on the ion drag force

N.Kh. Bastykova*, S.K. Kodanova, T.S. Ramazanov, Zh.A. Moldabekov

Institute of Experimental and Theoretical Physics, Al-Farabi Kazakh National University, Almaty, Kazakhstan

Knowing the magnitude of the ion drag force over a wide range of plasma parameters is necessary for understanding many processes in space and laboratory dusty plasmas. The strength of ion entrainment is responsible for the formation of voids (free regions) in experiments in the microgravity condition, responsible for the rotation of dust structures (clusters) in the presence of a magnetic field, and affects the dispersion of low-frequency oscillations [1].

Numerical calculations of the momentum transfer cross section for a wide range of parameter values β ($0.1<\beta<10^3$) for attractive and repulsive Yukawa interaction potentials are carried out in [2]. The results obtained for the momentum transfer cross section can be formulated as follows: the momentum transfer cross section for the attractive potential is always larger than the cross section for the repulsive potential. In papers [2-3], the ion drag force acting on the dust particle was obtained on the basis of the Yukawa potential and on the basis of the OML theory.

In this paper, the effect of the polarization of dust particles on the ion drag force and on the scattering of an ion around a dust particle was investigated. It is shown that for strong interactions ($\beta>>1$) the effect of the polarization effect is small, it arises only for weak interactions ($\beta<1$). The ion drag (orbit) force acting on the dust particle is obtained on the basis of the effective potential, which takes into account the polarization of the dust particles [4-5].

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* email: bastykova_nuriya@physics.kz

Quasi-Isentropic Compressibility of Deuterium at Pressure Region of ~12 Tpa

M. A. Mochalov[*1], R. I. Il'kaev[1], V. E. Fortov[2], A. L. Mikhailov[1], V. A. Arinin[1], A. O. Blikov[1], V. A. Komrakov[1], I. P. Maksimkin[1], V. A. Ogorodnikov[1], A. V. Ryzhkov[1]

[1] Russian Federal Nuclear Center All-Russia Research Institute for Nuclear Physics, Sarov, Nizhegorodskaya oblast, 607188 Russia
[2] Joint Institute for High Temperatures, Russian Academy of Sciences, Moscow, 125412 Russia

We report on the experimental results on the quasi-isentropic compressibility of a strongly nonideal deuterium plasma compressed to the density ρ ≈ 10 g/cc by pressure P = 11400 GPa (114 Mbar) on a setup of spherical geometry. We describe the characteristics of the experimental setup, as well as the methods for the diagnostics and interpretation of the experimental results.
The trajectory of metal shells that compress the deuterium plasma was detected using powerful pulsed X-ray sources with a maximal electron energy of up to 60 MeV. The value of the plasma density ρ ≈ 10 g/cc, was determined from the measured value of the shell radius at the instant that it was stopped. The pressure of the compressed plasma was determined using gasdynamic calculations taking into account the actual characteristics of the experimental setup.

* email: mochalov65.m@yandex.ru

A New Scheme for High-Intensity Laser-Driven Electron Acceleration in a Plasma

S. P. Sadykova[1] , A. A. Rukhadze [2],
[1] Forschungszentrum Juelich - Juellich Supercomputing Centre (JSC)
[2] Prokhorov General Physics Institute, RAS, Vavilov Street 38, Moscow, 119991, Russia

During the past few decades plasma accelerators have attracted increasing interest of scientists from all over the world due to its compactness, much cheaper construction costs compared to those for conventional one and various applications ranging from high energy physics to medical and industrial applications. 3 M€ of funding have been awarded to 16 laboratories and universities from 5 EU member states within the European Union's Horizon 2020 programme – **EuPRAXIA** (European Plasma Research Accelerator with eXcellence in Applications). They are joined by 16 associated partners that make additional in-kind commitments. The goal of this ambitious project is to produce a conceptual design report for the worldwide first high energy plasma-based accelerator that can provide industrial beam quality and user areas.

At the Forschungszentrum Jülich in a frame of the JuSPARC project it is planned to establish a short-pulse, petawatt laser facility (power above 1 PW with pulse durations in the 10 fs range). This will be utilized to produce ultra-short pulsed X-rays based on the laser-driven electon acceleration concept, providing high-brightness probes for materials science and biology applications relying on both high spatial and temporal resolution. In the standard laser-driven particle accelerator, a short laser pulse excites a trailing plasma wave that can trap and accelerate electrons to high energy with the very high electric field gradient. Unlike light sources of comparable wavelength such as the planned XFEL (X-ray free electron laser) at DESY, the laser-driven techniques potentially offer a much more compact and convenient operating environment with obvious advantages for FZJ-based research teams. Owing to the complex, nonlinear nature of the latter, only **detailed numerical modelling and theoretical analysis** will be able to provide the quantitative guidance necessary to optimize the beam characteristics required for a particular application. Establishment of collaboration between the various European institutes and FZJ in a frame of the **JuSPARC** and **EuPRAXIA** projects could be mutually beneficial.

The idea to accelerate the charged particles in a plasma medium using collective plasma fields belongs to Budker, Veksler, and Fainberg. Later on, another acceleration schemes were proposed including the laser plasma acceleration. In our earlier work we proposed a A New Scheme for High-Intensity Laser-Driven Electron Acceleration in a Plasma [1]. In our present work, we discuss and study further the suggested scheme taking into account different factors which can influence for example the plasma instability, consequently, the plasma wave amplification.

Due to the stimulated scattering of a laser pulse by electrons the longitudinal plasma wave is generated. When the instability increases the much higher magnitudes of electric fields compared to the conventional accelerators can be gained. It is known that the wakefield generating instability induced by the stimulated back-scattering (backwards the laser pulse) has a maximum increment. However, this acceleration scheme is not suitable for particle acceleration because due to the short laser pulse the scattering wave and laser wave soon get out of phase. Since the wave vector of a plasma wave $\vec{k}_p$ is equal to the double magnitude of that of a laser pulse ($\vec{k}_p \simeq 2\omega_0/c$), the phase velocity of a plasma wave is quite low. Due to this fact the wave leaves behind both the laser and the backward-scattered waves getting localized at the back to the front of the laser pulse. As a result the plasma wave gets soon out of the acceleration phase with the laser wave and the relativistic electron beam, injected into the plasma, gets soon out of a phase with the plasma wave what halts the acceleration process. Due to the laser forward scattering a forward wave is generated. In this case, the plasma wave and the injected electrons can stay in acceleration phase for a much longer time. We determine additional conditions, not considered earlier, for such a resonance at which the maximum electron acceleration energy can be gained, for ex. the plasma temperature, relativistic effects, make an estimation of a plasma, injected electron Bunch parameters, maximum amplitude of the generated electric field and assist them with simulations using the EPOCH-code. As the basis parameters and for comparison we use those set in the planned plasma acceleration experiment at SPARC LAB facility of INFN-LNF, Frascati, Italy, with external electron injection [2].

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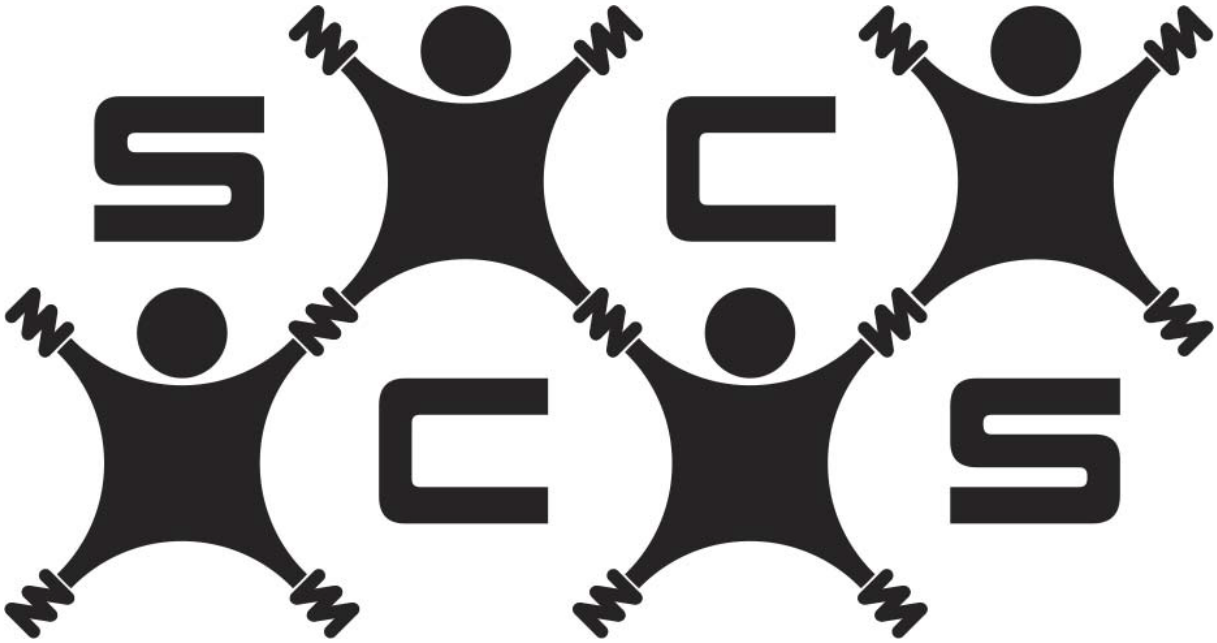
List of participants



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Acknowledgement: The local organizers thank Tim Schoof for providing his LaTeX-knowhow and help preparing this book of abstracts.

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