SCCS 2014

International Conference on
Strongly Coupled Coulomb Systems

July 27th-August 1st
Santa Fe, New Mexico, USA

SCCS 2014 is hosted by:

SCCS IAB

Sponsors:

Table of Contents

WELCOME

Dear SCCS 2014 Participants:

Let us be the first to welcome you to Strongly Coupled Coulomb Systems (SCCS) 2014 and Santa Fe. The community has come forward with an exciting set of talks and posters. The series of Strongly Coupled Coulomb Systems conferences are devoted to providing a forum where physicists, material scientists, chemists, engineers and mathematicians from a variety of disciplines can communicate across wide disciplinary boundaries. Our goal is to provide a relaxing, yet invigorating atmosphere in which to have productive scientific exchanges.

The Local Organizing Committee (LOC) and the Program Committee (PC), in consultation with the International Advisory Board (IAB), have put together a conference designed to stimulate discussion and interaction among attendees. The talks have been selected to give attendees both an overview of the latest scientific research in strongly coupled Coulomb systems in a wide variety of fields, and specialized detail. In keeping with SCCS tradition, posters are an equally important part of the program. Before each poster session, poster presenters will be giving everyone a brief one-minute overview of their posters.

We have also included time for discussion and for excursions into the local area. On Wednesday each participant will have an opportunity to join either a half-day excursion to Bandelier National Monument or a tour through the Santa Fe art scene. The two groups will regroup and meet for an authentic New Mexican dinner in the historic old town of Chimayo.

Finally, our deepest thanks go out to the members of the LOC, PC and IAB for the many hours of hard work that they put into organizing this conference. On the LOC, Lorin Benedict, Bob Cauble, Rip Collins, Rob Rudd, Liam Stanton and Heather Whitley did an incredible job organizing the conference, which was a second full-time job on top of their already busy schedules. From the LOC, Jim Glosli deserves a special note of thanks. He went beyond the call of duty in coordinating all of the events and keeping us within budget. On the PC, David Neilson, Angel Alastuey and Ronald Redmer did a fabulous job putting together an exciting program, and it was a joy working with them. We owe the IAB a special note of thanks for providing invaluable feedback and advice. Of particular note, Michael Bonitz was a wonderful sounding board for our ideas. Michael Fisher and the National Academy of Sciences was a font of wisdom regarding visa concerns for our foreign colleagues. In addition, Michael Fisher provided a keen critical eye in looking over our draft plans, program and website when it was needed. Finally, the New Mexico Consortium, under the leadership of Monica Wu, provided outstanding event planning during a time of challenging regulatory demands.

We are here to make this the best SCCS conference to date; let us know if there is anything we can do to help. We hope you find the conference stimulating and challenging, but also fun - enjoy!

Frank R. Graziani, Local Organizing Committee Chair
Michael S. Murillo, International Advisory Board Chair

Committees

International Advisory Board

Michael S. Murillo, Chair, Los Alamos National Laboratory
Angel Alastuey, École Normale Suprieure de Lyon
Jose Alejandre, Universidad Autonoma Metropolitana-Iztapalapa
John Bollinger, National Institute of Standards and Technology at Boulder
Michael Bonitz, University Kiel
Robert Cauble, Lawrence Livermore National Laboratory
David M. Ceperley, National Center for Supercomputing Applications, UIUC
Gilles Chabrier, cole Normale Suprieure de Lyon
Jean Clerouin, CEA/Limeil-Valenton, Villenueve St. Georges
Alan DeSilva, Institute for Research in Electronics & Applied Physics - University of Maryland
Claude Deutsch, Laboratoire de Physique des Gaz et des Plasmas-Université Paris
Zoltan Donko, Research Institute for Solid State Physics & Optics, HAS
Dan Dubin, University of California, San Diego
James Dufty, University of Florida
Vladimir Filinov, RAS/Institute of High Energy Density, Moscow
Michael Fisher, Institute for Physical Science & Technology, University of Maryland
Vladimir Fortov, RAS/Institute of High Energy Density, Moscow
Kenneth Golden, University of Vermont
John Goree, University of Iowa
Ulrich Heinz, Ohio State University
Friedrich Hensel, Philipps-Universität Marburg
Gabor Kalman, Boston College
M. Howard Lee, University of Georgia
Hartmut Löwen, Heinrich-Heine-Universität Düsseldorf
Yuri Lozovik, RAS/Institute of Spectroscopy, Moscow
Yitzhak Maron, Weizmann Institute of Science
Gregor Morfill, Max-Planck-Institute for Extraterrestrial Physics
David Neilson, Università degli studi di Camerino
Francois Peeters, University of Antwerp
Vittorio Pellegrini, Scuola Normale Superiore, Pisa
David Pines, Institute for Complex Adaptive Matter
Rudolph Podgornik, National Institute of Health & University of Ljubljana
Ronald Redmer, Universität Rostock
Gerd Roepke, Universität Rostock
Marlene Rosenberg, University of California, San Diego
Manfred Schlanges, Universität Griefswald
Gaetano Senatore, Università di Trieste, Trieste
Hiroo Totsuji, Okayama University
Giovanni Vignale, University of Missouri-Columbia
Xiaogang Wang, University of Beijing

Executive Committee

Michael Bonitz, Chair, Kiel
Vladimir Fortov, RAS
John Goree, Univ. Iowa

Program Committee

David Neilson, Chair, Camerino
Ronald Redmer
Angel Alastuey
Frank Graziani, *ex officio*
Michael S. Murillo, *ex officio*

Local Organizing Committee

Frank Graziani, Chair, LLNL
Michael S. Murillo, LANL
Lorin Benedict, LLNL
Jim Glosli, LLNL
Heather Whitley, LLNL
Liam Stanton, LLNL
Rip Collins, LLNL
Robert Cauble, LLNL
Rob Rudd, LLNL

Conference History

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

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

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

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

General Information

For the most updated and detailed information, see the conference website: www.sccs2014.net

Internet access will be available to attendees and guests of the La Fonda. The network password is: **freedom1** (all lower-case). Internet and printing will also be available at the La Fonda business center, which is located in the North Wing of the 2nd floor.

Onsite Points of Contact

Shannan Yeager
Phone: (803) 617-8722
e-mail: syeager@newmexicoconsortium.org

Carrie Talus
Phone: (505) 695-6511
e-mail: ctalus@newmexicoconsortium.org

Susan Espinoza
Phone: (505) 927-0268
e-mail: sye@lanl.gov

Transportation to/from the Airport:

Albuquerque International Airport (http://www.cabq.gov/airport/) is the closest major airport to Santa Fe. The airport is serviced by all major rental car companies (http://www.cabq.gov/airport/parking/car-rental). In addition, shuttle services are available (http://www.sandiashuttle.com/) that will transport you to and from the airport and the local hotels in Santa Fe. Santa Fe (http://santafe.org/) is approximately 66 miles and a little over an hour drive from the airport.

Presentation Information

All speakers should plan their content so that it follows the guidance described below.

- Contributed talks: 15 minutes (12 min presentation + 3 min for questions)
- Invited talks: 30 minutes (25 min presentation + 5 min for questions)
- Keynote talks: 45 minutes (40 min presentation + 5 min for questions)
- All session chairs will be instructed to keep us on time.

Oral Presenter Instructions

SCCS2014 will make available to all speakers both a MAC and a PC to show your slides. We will be presenting all talks from our computers. PDF is the preferable format, but we will accept PowerPoint. We would like to have your slides NO LATER THAN 5:00 PM THE DAY BEFORE YOU SPEAK, so we can load them on to our computers.

All talks should be emailed to sccs2014usa@gmail.com with the subject heading "SCCS2014 Slides". Please cc Frank Graziani at graziani1@llnl.gov.

If necessary, we can load your talk via a thumb drive onto our laptop prior to the start of your session. We will also have a MAC and PC available for you to preview your talk. The location of the MAC and PC for previewing will be specified in the program.

Poster Presenter Instructions

In order to advertise the posters, we have allocated time in the program called "Poster Session Oral Introductions". All posters will be asked to identify a single spokesperson. That person is asked to introduce their work on the day their poster is scheduled. All poster presenters will be allocated no more than 1 minute to invite people to their poster.

We are asking for all poster presenters to create 1 slide addressing:

- Title of the poster
- Authors and affiliated institutions
- A bullet or two addressing : Purpose of the work or key result.

If you have not done so already, email your single slide to sccs2014usa@gmail.com with the subject heading "Poster Invitation" as soon as possible. In addition, please cc Frank Graziani at graziani1@llnl.gov.

For the Poster Session "Oral Introductions" session, we will store all 1 slide introductions on our laptop and ask all presenters to come to the front of the room so we can minimize the time between speakers.

For the actual poster presentation, poster boards will be 4 feet by 8 feet. We will supply pins to secure your poster. Your poster may be many small sheets, one large sheet or any combination so that it does not exceed the 4×8 size. You are responsible for printing out your poster and bringing it to the room.

Excursion Information

On Wednesday, July 30, attendees will be given the option to attend one of two excursions; both of which will be followed by a special tour of El Santuario de Chimayó and a dinner at Rancho De Chimayó Restaurante.

Cost:
The dinner will be free of charge for all conference attendees. We assume all conference attendees would like to attend. Please check in with onsite registration desk and let our onsite administrator know by noon on Monday (July 28) if you are NOT going to attend. If you would bring any guests, please notify our onsite administrator, as we need to reserve their bus seats in advance. The dinner costs for guests is $24.75/person (fixed rate including all). You will pay for your guests at the restaurant.

Transportation:
People who are going on the Bandelier excursion will be dropped off at El Santuario de Chimayó around 5:30 PM. After dinner, a bus will take you back to La Fonda by 9:30 PM. If you DO NOT want to participate in the tour and following dinner, please notify our onsite administrator by noon on Monday. On Wednesday, make sure you stay on the bus, and you will be dropped off at La Fonda around 6:30 PM.

Participants who choose to go on the Museum Hill and Canyon Road tour will be dropped off at El Santuario de Chimayó around 5:30 PM to join the Bandelier group. If you DO NOT want to go, please notify our onsite administrator by noon on Monday. On Wednesday, make sure you ask the driver to drop you off at La Fonda before the bus departs for Chimayó.

Attendees who don't want to participate in any excursion but would like to join the El Santuario de Chimayó tour and the following dinner, please notify our onsite administrator by noon on Monday, and wait outside of La Fonda at 4:40 PM (excursion loading/unloading area) on Wednesday, and you will be picked up by bus heading to Chimayó.

Option A: Bandelier National Monument Tour

Times:

- 1:15 PM Loading/get boxed lunch
- 1:30 PM Leave Santa Fe
- 2:30 PM Arrive at Bandelier
- 4:30 PM Leave Bandelier park
- 5:30 PM Arrive at Chimayó
- 8:45 PM Leave Chimayó

- 9:30 PM Arrive at La Fonda

Transportation, guides, park entrance fees, bottled water on board and gratuities will be paid for all conference registrants who reserved their seats. If you are planning to bring any guests, it is $55/seat and please reserve seats and make payment via online registration form.

Bandelier National Monument protects over 33,000 acres of rugged but beautiful canyon and mesa country as well as evidence of a human presence here going back over 11,000 years. Petroglyphs, dwellings carved into the soft rock cliffs, and standing masonry walls pay tribute to the early days of a culture that still survives in the surrounding communities.

Please note that Bandelier National Monument tour requires a short hike and during warm summer time it could be more challenging than you think. Be prepared to dress comfortably, bring water and wear sunblock.

Option B: Museum Hill and Canyon Road Gallery Tour

Times:

- 1:15 PM Loading/get boxed lunch
- 1:30 PM Head to museum hill
- 3:30 PM Drive to the top of Canyon Road
- 4:30 PM Drive back to La Fonda.
- 4:45 PM Arrive at La Fonda. (Guests who don't go to Wed. dinner will be dropped off here, and guests who were not in any of the excursion groups will board the bus and drive to Chimayó for dinner)
- 5:30 PM Arrive at Chimayó and join in the bigger group
- 8:45 PM Leave Chimayó
- 9:30 PM Arrive at La Fonda

Transportation, guide, bottled water on board and gratuities are covered for all conference registrants who reserved their seats. If you are planning to bring any guests, it is $55/seat and please reserve seats and make payment via online registration form.

Extra costs: Participants are responsible for purchasing their own museum passes.

Canyon Road Art Galleries

Santa Fe's premier gallery district, Canyon Road is located just a mile from the plaza . Featuring more than a hundred art galleries in a mile-long stretch. Works by Native American artists,

as well as contemporary Santa Fe craftspeople offer everything from paintings and sculpture to jewelry, crafts, furniture, glasswork, photography, and fiber arts. For more information, visit www.canyonroadarts.com.

Museum Hill

Museum Hill in Santa Fe, New Mexico offers a central destination for exploring some of the city's finest museums and some of the world's greatest collections of Native American art and artifacts. The Museum of Indian Arts & Culture, the Wheelwright Museum of the American Indian, the Museum of Spanish Colonial Art, and the Museum of International Folk Art are the major institutions located on Santa Fe's Museum Hill. More information can be found here.

Proceedings Information

The conference proceedings for SCCS2014 will be published in the journal Contributions to Plasma Physics (CPP). Each article will undergo peer-review. A minimum article length of 6 journal pages will be imposed, in an effort to ensure that each contribution is reasonably self-contained (but note that the density of words in this journal is much lower than, say, Physical Review, for instance). Submission will be through the CPP website:

http://onlinelibrary.wiley.com/journal/10.1002/%28ISSN%291521-3986/homepage/instructions.html

The "Instructions to the Authors" in the above link should be followed. When submitting their manuscripts, authors should select as the type of article "SCCS2014 special issue". Authors are strongly encouraged to use Latex and the style files found at that page with figures in ps or pdf format. This will substantially shorten the time from submission to online publication.

Poster Competition

We are pleased to announce that the publisher of Contributions to Plasma Physics (Wiley VCH) has agreed to finance three cash awards for best posters. We have decided to give out one award in each of the following three categories:

- Best student poster
- Best experimental poster
- Best computational or theoretical poster

The winning posters will be announced at the Banquet on Thursday.

July 27 (Sunday)

15:30–19:30 **Check-in/On-Site Registration – Mezzanine Level**

17:30–19:30 **Opening Reception – La Terraza Room**

July 28 (Monday)

08:30–18:30 **Scientific Progam – Lumpkin Ballroom South (Talks) and Ballroom North (Posters)**

08:30–08:45 **Welcome – Michael Murillo and Frank Graziani**

08:45–09:30 Keynote **G. W. Collins**, "Exploring planets to stars at the National Ignition Facility, today's microphysics observatory"

09:30–10:00 Invited **N. Nettelmann & J. J. Fortney**, "Jupiter and Saturn models with compositional gradient"

10:00–10:15 Contributed **M. P. Desjarlais & A. D. Baczewski**, "Accurate entropies for liquids from MD simulations"

10:15–10:45 **Coffee Break – Lumpkin Ballroom North**

10:45–11:00 Contributed **Laura Johnson, Stephanie Hansen & David Hammer**, "Atomic Processes in Plasmas Investigation of X-Ray Thomson Scattering Using A Statistical Approach"

11:00–11:15 Contributed **Andreas Becker, Winfried Lorenzen, Jonathan J. Fortney, Nadine Nettelmann, Manuel Schottler & Ronald Redmer**, "Modeling Brown Dwarfs using ab initio equation of state data"

11:15–11:30 Contributed **M. Bethkenhagen, S. Hamel & R. Redmer**, "Superionic water-ammonia mixtures"

11:30–11:45 Contributed **Paul E. Grabowski, Michael P. Surh, David F. Richards, Frank R. Graziani & Michael S. Murillo**, "Molecular Dynamics Simulations of Classical Stopping Power: Testing and Improvements of Collision Operators"

11:45–12:00 Contributed **Jiaolong Zeng, Jiayu Dai & Jianmin Yuan**, "Radiation transfer of ultra-intense x-ray laser pulses through solid state density of aluminium"

12:00–12:30 Invited **Dongdong Kang, Jiayu Dai, Zengxiu Zhao, Jiaolong Zeng & Jianmin Yuan**, "Structures and dynamics in dense matter"

12:30–14:30 **Lunch and Informal Discussions**

14:30–15:15 Keynote **Jérôme Daligault**, "Classical Kinetic Theory of Strongly Coupled Coulomb Systems: Coveted, Elusive, Gripping"

15:15–15:30 Contributed **J. L. Belof & J. L. DuBois**, "Variational Path Integral Monte Carlo Approach for Warm Dense Matter"

15:30–15:45 Contributed **Charles Starrett, Jérôme Daligault & Didier Saumon**, "Pseudo-atom molecular dynamics"

15:45–16:00 Contributed **V. Filinov, Yu. Ivanov, M. Bonitz, V. Fortov & P. Levashov**, "Quantum simulation of thermodynamic and transport properties of quark - gluon plasma"

16:00–16:15 Contributed **A. D. Baczewski, L. Shulenburger, M. P. Desjarlais & R. J. Magyar**, "Dielectric Response in Extreme Conditions Using Time-Dependent Density Functional Theory"

16:15–16:30 **Coffee Break – Lumpkin Ballroom North**

16:30–18:30 **Poster Session 1 – Lumpkin Ballroom North**

Poster 1.01 **A. Calisti, S. Ferri & B. Talin**, "Ionization potential depression in hot dense plasmas through a pure classical model"

Poster 1.02 **D. Saumon, C. E. Starrett & J. O. Daligault**, "The calculation of diffusion coefficients in warm and hot dense matter"

Poster 1.03 **Dongdong Kang, Jiayu Dai, Huayang Sun & Jianmin Yuan**, "Nuclear quantum effects on the structure and dynamics of dense hydrogen"

Poster 1.04 **H. D. Whitley, W. E. Alley, J. I. Castor, A. Szoke, J. Nilsen & H. E. DeWitt**, "Solidification and Screening Enhancement in Asymmetric Binary Ionic Mixtures"

Poster 1.05 **Huayang Sun, Jiayu Dai, Dongdong Kang, Jiaolong Zeng & Jianmin Yuan**, "Temperature-dependent interatomic potential based on ab initio simulation"

Poster 1.06 **I. M. Saitov**, "DFT calculation of plasma frequency and free electron density in dense xenon plasma"

Poster 1.07 **In Gee Kim & Michael S. Murillo**, "Quantum Statistical Potentials for Electron-Ion Plasmas in the Random-Phase Approximation"

Poster 1.08 **Jérôme Daligault**, "A step towards a kinetic theory of strongly coupled Coulomb systems."

Poster 1.09 **K. N. Dzhumagulova, E. O. Shalenov & T. S. Ramazanov**, "Influence of dynamic screening on the scattering cross sections of the particles of the dense semiclassical plasma"

Poster 1.10 **L. G. Stanton & M. S. Murillo**, "Impact of Screening and Ionization on Coulomb Coupling in Strongly Coupled Plasmas"

Poster 1.11 **M. T. Gabdullin, T. S. Ramazanov, T. N. Ismagambetova & G. B. Ahtanova**, "Thermodynamic Properties of Semiclassical Partially Ionized Hydrogen and Helium Plasmas"

Poster 1.12 **Mayur Jain, John Verboncoeur & Andrew Christlieb**, "Electrostatic particle based modeling for simulation of strongly coupled plasmas"

Poster 1.13 **N. Kh. Bastykova, S. K. Kodanova & T. S. Ramazanov**, "Two-dimensional distribution of plasma parameters in the He/H2 gas mixtures in a stratified glow discharge"

Poster 1.14 **R. Bredow, T. Bornath, W. -D. Kraeft, M. W. C. Dharma-wardana & R. Redmer**, "Classical-map hypernetted chain calculations for multi-component plasmas"

Poster 1.15 **R. Piron, T. Blenski, C. Caizergues & B. Cichocki**, "Variational Average-Atom in Quantum Plasma - review and recent progress"

Poster 1.16 **Scott D. Baalrud, Kim Rasmussen & Jérôme Daligault**, "A Practical way to Extend Plasma Transport Theory to Strong Coupling"

Poster 1.17 **V. Ballenegger**, "On the origin of the surface term in the Ewald potential for periodic charged systems"

Poster 1.18 **Yu. V. Arkhipov, A. B. Ashikbayeva, A. Askaruly & I. M. Tkachenko**, "Dynamic collision frequency of Kelbg-pseudopotential-modelled plasmas"

Poster 1.19 **Zh. A. Moldabekov, P. Ludwig, M. Bonitz & T. S. Ramazanov**, "Dynamically screened ion potential in the presence of streaming degenerate electrons"

08:25–08:30 **Announcements**

08:30–09:15 **Silke Ospelkaus**, "Towards dipolar quantum many-body physics with ultracold polar molecules"
Keynote

09:15–09:45 **Kevin S. Bedell & James D. Stokes**, "The Virial Theorem for Dirac Materials"
Invited

09:45–10:00 **Louis Harbour, M. W. C. Dharma-wardana, Dennis Klug & Laurent Lewis**, "Phonons in
Contributed two-temperature states of solid Aluminum and Gold"

10:00–10:15 **S. B. Hansen, C. E. Starrett, D. Saumon, M. Desjarlais, A. Ng & V. Recoules**,
Contributed "Consistency in transport calculations for strongly coupled plasmas"

10:15–10:45 **Coffee Break – Lumpkin Ballroom North**

10:45–11:15 **Khandker Quader & Michael Widom**, "Pressure–Driven Lifshitz Transitions in 122-Pnictides"
Invited

11:15–11:30 **D. Cebulla & R. Redmer**, "High pressure phase diagram for MgO"
Contributed

11:30–11:45 **G. E. Norman, I. M. Saitov & V. V. Stegailov**, "Plasma-Plasma and Liquid-Liquid First-Order
Contributed Phase Transitions"

11:45–12:00 **E. R. Meyer, L. A. Collins, J. D. Kress & C. Ticknor**, "Molecular Mixtures of Relevance to
Contributed Planetary Interiors"

12:00–12:15 **Sebastien Hamel**, "First-principles evaluation of the entropy of silicon dioxide and
Contributed thermodynamics of giant impacts"

12:15–12:30 **Robert E. Rudd & Tomorr Haxhimali**, "Species Diffusion in Plasma Mixtures"
Contributed

12:30–14:30 **Lunch and Informal Discussions**

12:30–14:30 **Working IAB Luncheon – Stiha Room**

14:30–15:00 **L. X. Benedict**, "MD simulations and kinetic theory calculations of energy and particle transport
Invited processes in plasmas"

15:00–15:15 **P. Mabey, N. J. Hartley, H. W. Doyle, C. R. D. Brown, A. P. L. Robinson & G. Gregori**,
Contributed "Modelling fast electron transport in warm dense carbon"

15:15–15:30 **Andreas Markmann, Michael S. Murillo, Victor S. Batista & Frank Graziani**, "Toward
Contributed Quantum Molecular Dynamics Of The Electron Density with Classical Nuclei"

15:30–15:45 **D. Charkraborty, J. W. Dufty, V. V. Karasiev & S. B. Trickey**, "Proper Finite-temperature
Contributed Density Functionals and Their Computational Implementation"

15:45–16:00 Contributed **Yu. V. Arkhipov, A. B. Ashikbayeva, A. Askaruly, A. E. Davletov, S. Syzganbaeva & I. M. Tkachenko**, "Dense plasma dynamic structure factor simulation data vs. the method of moments"

16:00–16:15 Contributed **M. Bussmann, T. Kluge, L. Huang & T. E. Cowan**, "The Helmholtz Beamline at XFEL Probing solid density laser-plasma physics with XFELs on the femtosecond scale"

16:15–16:30 **Coffee Break – Lumpkin Ballroom North**

16:30–18:30 **Poster Session 2 – Lumpkin Ballroom North**

Poster 2.01 **D. Wendland, A. Alastuey & V. Ballenegger**, "Path Integral Monte Carlo calculations of internal partition functions for composite particles in quantum plasmas"

Poster 2.02 **F. R. Graziani, J. D. Bauer & M. S. Murillo**, "Kinetic Theory Molecular Dynamics and Hot Dense Matter"

Poster 2.03 **G. A. Pavlov**, "Nonlinear response theory of non-ideal charged and neutral matter"

Poster 2.04 **H. D. Whitley, D. M. Sanchez, S. Hamel, A. A. Correa & L. X. Benedict**, "Molecular Dynamics Simulations of Warm Dense Carbon"

Poster 2.05 **J. V. Stern & M. S. Murillo**, "Self-Diffusion in Weakly-to-Strongly Coupled Yukawa Systems"

Poster 2.06 **Kenneth I. Golden & Joshuah T. Heath**, "Hierarchy of Static Fluctuation-Dissipation Theorems for the Classical One-Component Plasma"

Poster 2.07 **L. G. Stanton & M. S. Murillo**, "A Gradient-Corrected, Analytic Screening Potential for Dense, Strongly-Coupled Plasmas"

Poster 2.08 **M. Rosenberg & G. J. Kalman**, "Waves in a Lennard-Jones Dusty Plasma Liquid"

Poster 2.09 **P. Magyar, Z. Donkó, G. J. Kalman & K. I. Golden**, "Linear and quadratic static response functions of 3D Yukawa liquids"

Poster 2.10 **Paul E. Grabowski**, "Understanding the Difference between Transport in Strongly Coupled Quantum and Classical Plasmas"

Poster 2.11 **S. A. Orazbayev, T. S. Ramazanov, M. K. Dosbolayev & M. Silamiya**, "Optical emission diagnostics of plasma in a gaseous mixture of RF discharge"

Poster 2.12 **S. K. Kodanova, T. S. Ramazanov & M. K. Issanova**, "Generalized Coulomb logarithm and energy loss of heavy particles in dense plasma"

Poster 2.13 **T. Ott, M. Bonitz & H. Löwen**, "2D One-Component and Binary Yukawa Systems in a Magnetic Field"

Poster 2.14 **Travis Sjostrom**, "Gradient Corrections to the Exchange-Correlation Free Energy"

Poster 2.15 **U. Zastrau, P. Sperling, G. Gregori, S. Toleikis, T. Döeppner, S. H. Glenzer & R. Redmer**, "Resolving Ultrafast Heating of Dense Cryogenic Hydrogen"

Poster 2.16 **V. E. Fortov, V. K. Gryaznov & I. L. Iosilevskiy**, "Thermodynamics of shock and isentropically compressed hydrogen and helium at megabar pressure range"

Poster 2.17 **Yan Feng, J. Goree, B. Liu, T. Intrator & M. S. Murillo**, "Superdiffusion of 2D Yukawa Liquids Due to a Perpendicular Magnetic Field"

Poster 2.18 **Yu. V. Arkhipov, A. B. Ashikbayeva, A. Askaruly, A. E. Davletov, D. Dubovtsev & I. M. Tkachenko**, "Enhancement of stopping power in dense two-component plasmas"

08:25–08:30 **Announcements**

08:30–09:15 Keynote **M. W. C. Dharma-wardana**, "A review of studies on Strongly-Coupled Coulomb Systems since the rise of DFT and the inaugural SCCS-meeting in 1977."

09:15–09:45 Invited **John Schliemann**, "Plasmons and Screening in Electron Systems with Internal Degrees of Freedom"

09:45–10:00 Contributed **M. Bonitz, S. Hermanns, C. Hinz, N. Schlünzeb & D. Lacroix**, "Relaxation dynamics of strongly correlated fermions in lattice systems"

10:00–10:15 Contributed **Daniel H. E. Dubin**, "Structure of Two-Dimensional Plasma Crystals in Anharmonic Penning Traps."

10:15–10:45 **Coffee Break – Lumpkin Ballroom North**

10:45–11:00 Contributed **James Dufty, Jeff Wrighton & Sandipan Dutta**, "Quantum Effects and Shell Structure for Confined Charges"

11:00–11:15 Contributed **C. Reichhardt & C. J. O. Reichhardt**, "Interacting Coulomb Systems on Periodic and Quasiperiodic Substrates: Applications in Dusty Plasmas, Soft Matter Systems, and Materials Science"

11:15–11:30 Contributed **S. De Palo & G. Senatore**, "Excitonic condensation in double-bilayer graphene"

11:30–11:45 Contributed **T. Schoof, S. Groth, A. Filinov & M. Bonitz**, "Thermodynamic properties of the homogeneous electron gas a Configuration Path Integral Monte-Carlo approach"

11:45–12:00 Contributed **Gautham Dharuman, Michael S. Murillo, John Verboncoeur & Andrew Christlieb**, "Strongly Coupled Ultracold Plasmas from Rydberg Blockaded Gas of Ultracold Atoms"

12:00–12:15 Contributed **B. B. Zelener, A. A. Bobrov, M. A. Butlitsky, S. Y. Bronin, D. R. Khikhlukha, V. A. Sautenkov, S. A. Sahakian, E. A. Manykin, B. V. Zelener & V. E. Fortov**, "Rydberg Matter and Ultracold Plasma."

12:15–12:30 Contributed **L. Silvestri, G. J. Kalman, Z. Donkó, P. Hartmann & H. Kählert**, "Fano-like resonances in strongly coupled Coulomb systems"

12:30–13:15 **Free Time**

13:15–13:30 **Board Buses for Excursions – on San Francisco Street near Garage Entrance**

13:30–16:30 **Conference Excursions**

16:30–17:30 **Board Buses and Travel to Chimayo**

17:30–18:00 **Tour El Santuario de Chimayo**

18:30–20:30 **Dinner at Rancho de Chimayo**

20:30–21:30 **Board Buses and Travel to Santa Fe**

08:25–08:30 **Announcements**

08:30–09:15 **T. Döppner**, "Fundamental Science Experiments on the National Ignition Facility"
Keynote

09:15–09:45 **G. Gregori**, "Laboratory Studies of Warm Dense Matter with High Power Lasers and 4th Generation Light Sources"
Invited

09:45–10:00 **Jean Clerouin, P. Arnault, G. Robert, C. Ticknor, J. D. Kress & L. Collins**, "Self-organization in dense plasmas: the Gamma-plateau"
Contributed

10:00–10:15 **Kai-Uwe Plagemann, Hannes Rüter, Thomas Bornath, Carsten Fortmann, Michael P. Desjarlais & Ronald Redmer**, "Static and dynamic structure factors for warm dense matter"
Contributed

10:15–10:30 **P. A. Zhilyaev & V. V. Stegailov**, "Two-temperature WDM of Al and Au: (quasi)thermodynamics and conductivity"
Contributed

10:30–11:00 **Coffee Break – Lumpkin Ballroom North**

11:00–11:30 **J. Boronat**, "Quantum dipolar gases"
Invited

11:30–11:45 **R. G. Bystryi & I. V. Morozov**, "Electron oscillations in nonideal cluster nanoplasmas"
Contributed

11:45–12:00 **M. Lyon & S. D. Bergeson**, "Using higher ionization states to increase the strong coupling of an ultracold neutral plasma"
Contributed

12:00–12:10 **Tribute to Hugh Dewitt by Gabor Kalman**

12:10–12:20 **Tribute to Forrest Rogers by Bob Cauble**

12:20–12:30 **Tribute to Bernard Jancovici by Angel Alastuey**

12:30–14:00 **Lunch and Informal Discussions**

14:00–14:30 **H. Kählert, T. Ott, A. Reynolds, M. Bonitz, G. J. Kalman & H. Löwen**, "Collective Excitations in Magnetized Strongly Coupled Plasmas"
Invited

14:30–14:45 **Subir K. Das, Young C. Kim & Michael E. Fisher**, "Charge-Charge Sum Rules in Near Critical Electrolytes"
Contributed

14:45–15:00 **P. Ludwig, H. Kählert, J. P. Joost, C. Arran, Zh. Moldabekov & M. Bonitz**, "Multiscale Simulation of Dust Clusters in a Strongly Magnetized Flowing Plasma"
Contributed

15:00–15:15 **E. Allahyarov, H. Löwen & A. Ivlev**, "Template controlled crystal growth in strongly coupled Coulomb plasma"
Contributed

15:15–15:30 **Chi Yang & Lin I**, "How does the cold dusty plasma liquid crack and heal under shear stress?"
Contributed

15:30–15:45 Contributed **A. E. Davletov, L. T. Yerimbetova, A. K. Ospanova & Ye. S. Mukhametkarimov**, "Polarization and finite size effects in correlation functions of dusty plasmas"

15:45–16:00 Contributed **T. S. Ramazanov**, "Strongly Coupled Complex Plasmas: Effective Potentials and Physical Properties"

16:00–16:15 **Coffee Break – Lumpkin Ballroom North**

16:15–18:00 **Poster Session 3 – Lumpkin Ballroom North**

Poster 3.01 **Bedros Afeyan**, "Nonlinear Kinetic Self-Organized Asymptotic States in High Energy Density Plasmas: Pump-Probe df/dv Diagnostics from the Visible to X-Rays"

Poster 3.02 **D. Batryshevi, T. Ramazanov, M. Dosbolayev, M. Gabdullin & S. Orazbayev**, "Method of separation of polydisperse particles in plasma of radio frequency discharge"

Poster 3.03 **David Michta, Liam G. Stanton, Mike Surh, Frank Graziani & Michael S. Murillo**, "A Non-Born-Oppenheimer Molecular Dynamics Method for Dense Plasmas"

Poster 3.04 **G. A. Pavlov, N. A. Suslov, V. M. Treushnikov, P. V. Garanin, Y. V. Pozdnyakov, V. V. Treushnikov & N. V. Zhidkov**, "Registration of clots images of dense plasma in the hard X-ray range"

Poster 3.05 **G. J. Kalman, Z. Donkó, P. Hartmann, K. I. Golden & L. Silvestri**, "Collective modes in binary systems: Coulomb vs. Yukawa"

Poster 3.06 **Gautham Dharuman, Guclu Yaman, Andrew Christlieb, John Verboncoeur & Michael S. Murillo**, "Molecular Dynamics Simulation with Momentum Dependent Potentials: Comparison of High Order Symplectic Integrators"

Poster 3.07 **H. D. Whitley, M. P. Desjarlais, C. R. Scullard, L. X. Benedict, J. I. Castor, M. S. Murillo & F. R. Graziani**, "Electronic transport properties of dense plasma"

Poster 3.08 **H. Kählert, G. J. Kalman & M. Bonitz**, "Kinetic approach to the dynamics of inhomogeneous strongly coupled plasmas"

Poster 3.09 **I. A. Valuev, N. A. Kazeev & I. V. Morozov**, "Simulation of Confined System of Interacting Fermions by Antisymmetrized Wave Packet Molecular Dynamics"

Poster 3.10 **I. Korolov, G. J. Kalman, L. Silvestri & Z. Donkó**, "Molecular Dynamics simulations of the classical one-component Coulomb plasma over the range $0.05 \leq \Gamma \leq 10000$"

Poster 3.11 **M. K. Dosbolayev, T. S. Ramazanov & A. U. Utegenov**, "Investigation of dusty plasma properties in various gas mixtures"

Poster 3.12 **M. M. Muratov, T. S. Ramazanov, K. N. Dzhumagulova & J. A. Goree**, "Pressure of the Dust Component Due to the Interaction"

Poster 3.13 **M. Marciante & M. S. Murillo**, "Shock Behavior in Strongly Coupled Dusty Plasmas"

Poster 3.14 **M. Moll, Th. Bornath, V. P. Krainov & M. Schlanges**, "Dynamics of Laser-excited Argon Clusters"

Poster 3.15 **M. Rosenberg, G. J. Kalman, P. Hartmann, Z. Donkó & S. Kyrkos**, "Waves in a Strongly Coupled 2D Superparamagnetic Dusty Plasma"

Poster 3.16 **T. Ott & M. Bonitz**, "Defining and Measuring the Coupling Strength in Coulomb and Yukawa Plasmas"

Poster 3.17 **V. E. Fortov & V. B. Mintsev**, "Quantum Bound for Shear Viscosity of Strongly Coupled Electron and Dusty Plasmas"

Poster 3.18 **Wei-Ting Chen & Jacob L. Roberts**, "Electron Oscillation Damping in Ultracold Neutral Plasmas"

Poster 3.19 **Y. A Ussenov, M. K. Dosbolayev, A. U. Utegenov & T. S. Ramazanov**, "Investigation of the electrons temperature in mixtures of noble gases"

Poster 3.20 **Yan Feng, John Goree & Bin Liu**, "Localized viscous heating observed in a two-dimensional strongly coupled dusty plasma"

18:00–18:30 **Free Time**

18:30–22:00 **Conference Banquet – La Terraza Room**
19:00–20:30 **Dinner Served**
20:30–21:00 **Poster and Student Awards**

08:25–08:30 **Announcements**

08:30–09:00 Invited **P. Hartmann, Z. Donkó, T. Ott, H. Kählert & M. Bonitz**, "Quasi-magnetization of rotating dusty plasmas"

09:00–09:15 Contributed **O. F. Petrov, V. E. Fortov, M. M. Vasiliev, Y. Tun, K. B. Stacenko, O. S. Vaulina, E. V. Vasilieva, E. M. Lisin & M. I. Myasnikov**, "Experimental Studies of Two-dimensional Melting in Dusty Plasma"

09:15–09:30 Contributed **C. Ticknor**, "First principles nonequilibrium plasma mixing"

09:30–09:45 Contributed **John Goree & W. D. Suranga Ruhunusiri**, "Is the compressibility positive or negative in a strongly-coupled dusty plasma?"

09:45–10:00 Contributed **Truell W. Hyde, Jay Kong & Lorin Matthews**, "Chains (Strings) in Complex Plasma"

10:00–10:30 Invited **C. P. Royall**, "Electrostatics in low-dielectric constant colloidal systems: ultra-long range, electroneutrality violation and self-induced anisotropy"

10:30–11:00 **Coffee Break – Lumpkin Ballroom North**

11:00–11:15 Contributed **P. M. Celliers, D. E. Fratanduono, D. H. Munro, T. R. Boehly, D. G. Hicks, J. H. Eggert & G. W. Collins**, "Experimental determination of the sound speed and Gruneisen coefficient of shock-compressed liquid deuterium"

11:15–11:30 Contributed **M. D. Knudson, M. P. Desjarlais, R. W. Lemke, K. Cochrane, A. Becker & R. Redmer**, "Pulsed power methods to access off-Hugoniot states in liquids"

11:30–11:45 Contributed **Y. Ping, J. King, O. L. Landen, R. Freeman, T. Boehly & G. W. Collins**, "Thermal conductivity measurements of CH and Be by refraction-enhanced x-ray radiography"

11:45–12:15 Invited **James N. Glosli, Dave F. Richards, Liam G. Stanton, Michael P. Surh & Michael S. Murillo,**, "The Role of high performance computing in Coulomb systems"

12:15–12:30 **Closing Remarks**

SCCS 2014
Abstracts

Monday, July 28th

Exploring planets to stars at the National Ignition Facility, today's microphysics observatory

G. W. Collins

Lawrence Livermore National Laboratory, Livermore, CA 94551, USA

New capabilities provide the first controlled laboratory-based experiments into the multi-Gbar pressure range, conditions exceeding the atomic unit of pressure (294 Mbar) and reproducing states existing deep inside stars, sub-stellar objects (e.g., brown dwarfs), and planets. Recent data are helping to build a framework for understanding and controlling hot-dense thermonuclear plasmas as well as ultra-dense highly degenerate matter where core as well as valance electrons control structure and bonding. We describe recent discoveries for such matter at extreme energy densities including new and unexpected phase transitions in dense solids and plasmas and surprisingly efficient energy transport in hot and dense plasmas.

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

Jupiter and Saturn models with compositional gradient

N. Nettelmann* and J. J. Fortney
University of California, Santa Cruz
Santa Cruz, CA 95064, U.S.A.

The giant planets in the solar system contain crucial information on its formation, one of the major scientific goals of ESA's Cosmic Vision plan and of NASA's Big Questions in Planetary Science. However, our understanding the H/He rich gas giants Jupiter and Saturn and the heavy element rich ice giants Uranus and Neptune is at the mercy of our knowledge on equations of state (EOS) and material properties like mixing, convection, and conductivity, and of course on astronomical observations.
Here we present and discuss new developments [1,2,3] in the modeling of the structure and evolution of Jupiter and Saturn that aim to explain Saturn's high luminosity [2] and Jupiter's atmospheric depletion in helium [3], respectively. In particular, these advanced models assume a compositional gradient and predict a zone of double diffusive instead of overturning convection.
According to our advanced models, if Jupiter's compositional gradient results from H/He phase separation and helium rain, the induced corrections to standard adiabatic, homogeneous models turn out to be small, in which case we continue to remain in the situation where the uncertainty in the H/He EOS still prevents a conclusion about whether Jupiter's interior is fully mixed or separated into a heavy-element poor outer envelope and a heavy-element-rich inner envelope as predicted by ab initio EOS based planetary structure models. On the other hand, if Jupiter and Saturn were born with a compositional gradient, they could be warmer and 2x more heavy-element rich than previously thought [1].
We emphasize the importance of high-precision laboratory experiments on the H EOS under planet interior conditions, of probing in-situ Saturn's atmosphere, and of numerical simulations on the behavior of planetary materials and of the dynamics of fluids.
*nadinen@ucolick.org

[1] J. Leconte, and G. Chabrier. *A new vision on giant planet interiors: Impact of double diffusive convection.* Astronomy & Astrophysics, **540** A20, (2012).

[2] J. Leconte, and G. Chabrier.. *Layered convection as the origin of Saturn's luminosity anomaly.* Nature geoscience, **6**, 347 (2013).

[3] N. Nettelmann, J. J. Fortney, and P. Garaud. *Layered double diffusive convection in Jupiter as a result of H/He demixing.* Submitted (2014).

Accurate entropies for liquids from MD simulations

M. P. Desjarlais* and A. D. Baczewski
Sandia National Laboratories†
Albuquerque, NM 87185, U.S.A.

The two-phase thermodynamic model[1] (2PT) provides a framework for the direct extraction of the entropy from long molecular dynamics simulations. The method is based on a decomposition of the translational and vibrational density of states into solid-like and gas-like components. The gas-like subsystem is modeled as a Carnahan-Starling hard-sphere liquid. The entropy contributions from the gas-like and solid-like subsystems are then computed with the appropriate Carnahan-Starling and quasi-harmonic weighting functions, respectively. In validation calculations with molecular dynamics simulations of the Lennard-Jones liquid, error levels of 1% to 5% were achieved.[1] A recent extension of the 2PT model employs a memory-function approach to characterizing the gas-like subsystem, providing for a more realistic representation of the diffusive dynamics, and resulting in a considerable increase of accuracy.[2] In comparisons with ambient pressure entropy data for a variety of liquid metals, errors at the level of 1% or less were demonstrated. In this work, we revisit the Lennard-Jones liquid with the memory function approach and compare calculated entropies to several Lennard-Jones equations of state and thermodynamic integrations over a wide range of densities and temperatures.
*mpdesja@sandia.gov

†Sandia National Laboratories is a multiprogram laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under Contract No. DE-AC04-94AL85000.

[1] S.-T. Lin, M. Blanco, and W. A. Goddard III, *The two-phase model for calculating thermodynamic properties of liquids from molecular dynamics: Validation for the phase diagram of Lennard-Jones fluids*, J. Chem. Phys. **119**, 11792 (2003).

[2] M. P. Desjarlais, *First-principles calculation of entropy for liquid metals*, Phys. Rev. E **88**, 062145 (2013).

Atomic Processes in Plasmas

Investigation of X-Ray Thomson Scattering Using A Statistical Approach

Laura Johnson[1], Stephanie Hansen[2], David Hammer[3].

[1] *Cornell University, Ithaca, NY, USA*
[2] *Sandia National Laboratories, Albuquerque, NM, USA*
[3] *Cornell University, Ithaca, NY, USA*

Abstract. We present a statistical method of computing x-ray Thomson scattering signals. This model uses average atom wave functions, which are computed in a spherically symmetric, self-consistent potential that vanishes at the Wigner-Seitz radius. The wave functions are used to obtain electron distributions for a statistical approach to computing the scattering signals. We compare the calculations to experimental data taken at Cornell's Laboratory of Plasma Studies.

Modeling Brown Dwarfs using ab initio equation of state data

Andreas Becker*[1], Winfried Lorenzen[1], Jonathan J. Fortney[2], Nadine Nettelmann[2],
Manuel Schöttler[1], and Ronald Redmer[1]
[1]Institut für Physik, Universität Rostock, D-18051 Rostock, Germany
[2]Department of Astronomy & Astrophysics, University of California, Santa Cruz, CA 95064

We present wide-range equations of state (EOS) for hydrogen and helium including accurate data derived from finite-temperature density functional theory molecular dynamics simulations for the warm dense matter regime using the VASP code [1]. These hydrogen/helium Rostock EOS (H/He-REOS) cover a wide range of temperatures (60 K - 10 MK) and densities ($1{\cdot}10^{-10}$ - 1000 g/cm^3) with a maximum error of 5% and reproduce data from high pressure experiments, for example the principal and precompressed Hugoniot curve and the 300 K isotherme derived from diamond anvil cell experiments, see [2] and [3]. Based on this ab initio data set we calculate interior models and mass-radius relations for Giant Planets and for the first time for Brown Dwarfs, which we compare with results derived using the EOS of Saumon, Chabrier and van Horn (SCvH) [4]. Assuming atmospheric conditions of P($\rho \sim 10^{-3}$ g/cm^3, T~1800 K) = 56 bar, we find for the Brown Dwarf Gliese 229b central conditions of P($\rho \sim 430$ g/cm^3, T~1.1 MK) = 220 Gbar, which differ by 10% from the SCvH results. These conditions can be probed at the National Ignition Facility, see [5].
*andreas.becker@uni-rostock.de

[1] G. Kresse and J. Furthmüller, Phys. Rev. B **54**, 11169 (1996).

[2] P. Loubeyre *et al.*, Phys. Rev. B **86**, 144115 (2012).

[3] A. Becker , N. Nettelmann, B. Holst, and R. Redmer, Phys. Rev. B **88**, 045122 (2013).

[4] D. Saumon, G. Chabrier, and H. M. van Horn, Astrophys. J. Suppl. Ser. **99**, 713 (1995).

[5] O.A. Hurricane *et al.*, Nature **506**, 343 (2014).

Superionic water-ammonia mixtures

M. Bethkenhagen[1,*], S. Hamel[2] and R. Redmer[1]
[1]University of Rostock, Institute of Physics
18051 Rostock, Germany
[2]Lawrence Livermore National Laboratory
Livermore, CA 94551, U.S.A.

The interior of the Giant Planets Uranus and Neptune contains large amounts of water, ammonia and methane (referred to as planetary ices). Many observable properties of these planets, such as luminosity, gravitational moments and magnetic fields, are thought to be determined by the physical and chemical properties of matter within this ice layer. Hence, the phase diagrams, equations of state and structural properties of these materials and their respective mixtures are of great interest. Especially the phase diagrams of water and ammonia gained much attention since Cavazzoni et al. [1] proposed superionic phases, which are characterized by highly mobile hydrogen ions in a lattice of oxygen and nitrogen ions, respectively. [2-4] For water, the influence of such a phase on the properties of the Giant Planets as well as on exoplanets has been discussed widely. [5,6]
Nevertheless, it is an open question how the properties of such a water layer change when another compound, e.g., ammonia is introduced. Considering a 1:1 mixture, we have performed ab initio simulations based on density functional theory using the VASP code [7] heating up structures which we had found from evolutionary random structure search calculations with XtalOpt [8]. We propose possible superionic water-ammonia structures present up to several Mbar in comparison to structures earlier found by Griffiths et al. [9] Moreover, we investigate the equation of state and transport properties of this mixture such as diffusion coefficients and electrical conductivities in order to compare with the pure compounds. These results are essential to construct new interior models for Neptune-like planets and to perform more realistic dynamo simulations.
*mandy.bethkenhagen@uni-rostock.de

[1] C. Cavazzoni et al., Science 283, 44 (1999).
[2] M. French et al., Phys. Rev. B 79, 54107 (2009).
[3] H. F. Wilson et al., Phys. Rev. Lett. 110, 151102 (2013).
[4] M. Bethkenhagen et al., J. Chem. Phys. 138, 234504 (2013).
[5] R. Redmer et al., Icarus 211, 798 (2011).
[6] L. Zeng and D. Sasselov, ApJ 784, 96 (2014).
[7] G. Kresse and J. Hafner, Phys. Rev. B 47, 558 (1993).
[8] D. C. Lonie and E. Zurek, Comput. Phys. Commun. 182, 372 (2011).
[9] G. I. G. Griffiths et al., J. Chem. Phys. 137, 064506 (2012).

Molecular Dynamics Simulations of Classical Stopping Power: Testing and Improvements of Collision Operators

Paul E. Grabowski*
University of California, Irvine, Irvine, CA 92697, U.S.A.
Michael P. Surh, David F. Richards, and Frank R. Graziani
Lawrence Livermore National Laboratory, Livermore, CA 94551, U.S.A.
Michael S. Murillo
Los Alamos National Laboratory, Los Alamos, NM 87545, U.S.A.

Molecular dynamics can provide very accurate tests of classical kinetic theory; for example, unambiguous comparisons can be made for classical particles interacting via a repulsive $1/r$ potential. The plasma stopping power problem, of great interest in its own right, provides an especially stringent test of a velocity-dependent transport property. We have performed large-scale (10^4 – 10^6 particles) molecular dynamics simulations of charged-particle stopping in a classical electron gas that span the weak to moderately strong intratarget coupling regimes. Projectile-target coupling is varied with projectile charge and velocity. Comparisons are made with disparate kinetic theories (both Boltzmann and Lenard-Balescu classes) and fully convergent theories to establish regimes of validity. Standard models break down at strong coupling and/or large projectile charge. We improve a Lenard-Balescu class type model via the inclusion of both target-target and target-projectile static local field corrections. This procedure worked well at moderate coupling ($\Gamma = 1$), but failed at large coupling ($\Gamma = 10$). A more successful approach was to improve the Boltzmann collision operator by including many-body physics in the cross section through the use of potentials derived from the Debye-Hückel formalism, Poisson-Boltzmann equation, and the hypernetted chain approximation. The last gave the best results, matching our molecular dynamics data, even for the $\Gamma = 10$, $Z = 10$ case. We improve the high-velocity behavior of the Boltzmann equation by extending a trick of Zwicknagel to strong coupling. We provide a useful fit to our results.
*paul.grabowski@uci.edu

[1] P.E. Grabowski, M.P. Surh, D.F. Richards, F.R. Graziani, M.S. Murillo *Molecular Dynamics Simulations of Classical Stopping Power.* Physical Review Letters, **111** 215002, (2013).

Radiation transfer of ultra-intense x-ray laser pulses through solid state density of aluminium

Jiaolong Zeng*, Jiayu Dai and Jianmin Yuan
Department of Physics, College of Science, National University of Defense Technology, Changsha Hunan, P.R. China, 410073

For weak radiation field, the radiative opacity and emissivity describe the optical properties of hot dense plasmas at local thermodynamic equilibrium (LTE) and non-LTE physical conditions. For ultra-intense x-ray laser pulses, however, the radiative properties of irradiated matter strongly depend on the intensity of lasers. We developed a theoretical formalism to deal with this problem by simultaneously solving the radiation transfer equation and the rate equation. The rate equation determines the evolution dynamics of charge state distribution (CSD) and level populations in the interaction of ultra-intense x-ray pulses with matter, while the radiation transfer equation determines the absorption of x-ray radiation. These two equations are coupled together. With the increase of intensity, the matter becomes transparent due to the empty K-shell states irradiated by the strong radiation field. The physical effects of Inner-shell resonant absorption were investigated on the CSD [1] and radiative properties. Moreover, the effects of direct double processes, such as direct double Auger decay [2,3], direct double photoionization, are investigated.

*jlzeng@nudt.edu.cn

[1] W.J. Xiang, C. Gao, Y.S. Fu, J.L. Zeng, and J.M. Yuan, Phys. Rev. A 86, 061401(R) (2012).
[2] J.L. Zeng, P.F. Liu, W.J. Xiang, and J.M. Yuan, Phys. Rev. A 87, 033419 (2013).
[3] J.L. Zeng, P.F. Liu, W.J. Xiang, and J.M. Yuan, J. Phys. B: At. Mol. Opt. Phys. 46, 215002 (2013).

Structures and dynamics in dense matter

Dongdong Kang, Jiayu Dai, Zengxiu Zhao, Jiaolong Zeng and Jianmin Yuan*
Department of Physics, National University of Defense Technology
Changsha, Hunan 410073, P. R. China.

Structures and dynamics of matter under extreme conditions are of importance in the fields of astrophysics, inertial confinement fusion, laser-matter interactions and dense plasmas [1,2]. Here, we focus on the behaviors of dense hydrogen and ice, which exist widely in giant planets. Traditional, ions are treated as classical particles. When the thermal wavelength of ions can be comparable to the ionic distances, the nuclear quantum effects (NQEs) will show their impact on the structures. Besides, quantum dynamics should be different from traditional classical dynamics, which will induce significant effects on the ionic scattering processes.
We develop the sampling method in path integral molecular dynamics, investigating the thermal properties of hydrogen and ice at high density up to the temperature of a few eV. For ice, by considering the nuclear NQEs, the phases around 100 GPa are consistent with the previous experiments. The oxygen K edge with its shift is sensitive to the order-disorder transition, and therefore can be applied to diagnose the dynamics of ice structures [3]. For dense hydrogen, the equation of states, ionic structures are strongly dependent on the NQEs. Most importantly, the quantum dynamics such as scattering determined electrical, thermal conductivity and ionic diffusion could be largely different from the classical results [4]. These quantum effects give new results of structures and show new quantum dynamics under the conditions of giant planet core and solar interior.

*jmyuan@nudt.edu.cn

[1] F. R. Graziani et al., High Energy Density Phys., 8: 105 (2012).

[2] J. M. McMahon, M. A. Morales, C. Pierleoni, and D. M. Ceperley, Rev. Mod. Phys.84,:1607 (2012).

[3] D. D. Kang, J. Y. Dai, H. Y. Sun, Y. Hou and J. M. Yuan. Quantum simulation of thermally-driven phase transition and oxygen K-edge x-ray absorption of high-pressure ice, Sci. Rep. 3, 3207 (2013).

[4]D. D. Kang et al. submitted.

Classical Kinetic Theory of Strongly Coupled Coulomb Systems: Coveted, Elusive, Gripping

Jérôme Daligault
Theoretical Division
Los Alamos National Laboratory, Los Alamos, NM 87545

Kinetic theory attempts to describe and predict the properties of gases and liquids in terms of the microscopic interactions and motions of its constituent molecules. For dilute gases, the Boltzmann equation has satisfactorily achieved the basic goals of kinetic theory. In spite of numerous efforts, no one has yet succeeded in deriving a comparable equation for dense gases and liquids, let alone strongly coupled Coulomb systems. In this talk, I will discuss the achievements that have been made in developing the kinetic theory of classical, strongly-coupled systems, and will describe recent proposals to break through that the challenges that have so far eluded us. I will put the problem into historical perspective and will make relevant connections to other areas of physics (liquid theory, quantum field theory, renormalization, closure problem...)

*daligaul@lanl.gov

Variational Path Integral Monte Carlo Approach for Warm Dense Matter

J.L. Belof* and J.L. DuBois
Lawrence Livermore National Laboratory
Livermore, CA 94551, U.S.A.

An accurate and predictive theoretical description of warm dense matter (WDM), the regime of degenerate and strongly coupled Coulomb systems, presents a grand challenge that is of long-standing interest. Path Integral Monte Carlo (PIMC) presents a direct numerical simulation approach to the quantum many-body problem that is, in certain limits, exact. Building on the work of Feynman and Kleinert[1,2] we present a new approach that extends the PIMC formalism to more strongly coupled systems for reduced computational cost. This new approach to warm dense matter provides certain advantages with regard to high performance computing architectures for the study of large systems and is demonstrated through a series of examples that include the spin polarized electron gas, dense hydrogen and helium, and warm dense carbon.

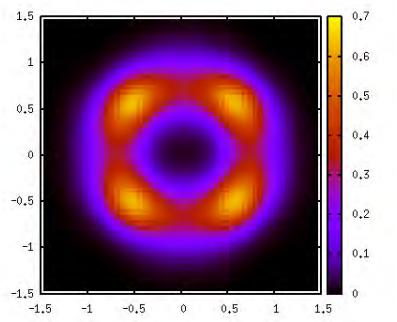


Figure 1: Path density resulting from a generalized 4-term path expansion for a free particle, where a trial density matrix has been optimized within the Feynman-Kleinert variational formalism.

*belof1@llnl.gov

[1] R.P. Feynman and H. Kleinert. *Effective Classical Partition Functions.* Phys. Rev. A., **34** 5080, (1986).

[2] M. Bachmann, H. Kleinert and A. Pelster. *Variational Perturbation Theory for Density Matrices.* Phys. Rev. A., **60** 3429, (1999).

The authors acknowledge funding from the U.S. Department of Energy, Basic Energy Sciences (Grant No. DE0GG02-07ER46470). Lawrence Livermore National Laboratory is operated by Lawrence Livermore National Security, LLC, for the U.S. Department of Energy, National Nuclear Security Administration under Contract DE-AC52-07NA27344.

Pseudo-atom molecular dynamics

Charles Starrett, Jérôme Daligault and Didier Saumon
Los Alamos National Laboratory

We have developed and new method for calculating the thermodynamics of warm dense plasmas. It combines an average atom-like approach to calculate the electronic structure of one pseudo-atom, with classical molecular dynamics (MD) for the ionic structure. Pair potentials for the MD simulations are generated using the pseudo-atom electron density. The result is a model in which both electronic and ionic structures of a plasma can be calculated rapidly and the resulting thermodynamics agree excellently with the much more expensive *ab initio* DFT-MD methods. We will present an outline of the new method and comparisons of pressures and internal energies with *ab initio* results.

Quantum simulation of thermodynamic and transport properties of quark - gluon plasma

V. Filinov*, Yu. Ivanov, M. Bonitz, V. Fortov, and P. Levashov
Joint Institute for High Temperatures, Russian Academy of Sciences,
Izhorskaya st. 13 Bd. 2, 125412 Moscow, Russia
NRC "Kurchatov Institute", Akademika Kurchatova pl., 123182, Moscow, Russia
Institute for Theoretical Physics and Astrophysics, Christian Albrechts University Kiel,
Leibnizstrasse 15, D-24098 Kiel, Germany

For quantum simulation of thermodynamic and transport properties of quark - gluon plasma (QGP) within unified approach we combine path integral and Wigner (in phase space) formulations of quantum mechanics. Thermodynamic properties of a strongly coupled quark-gluon plasma (QGP) of constituent quasiparticles is studied by a color path-integral Monte-Carlo simulations (CPIMC). For simulations we have presented QGP partition function in the form of color path integral with new relativistic measure instead of Gaussian one used in Feynman and Wiener path integrals. For integration over color variable we have also developed procedure of sampling color variables according to the group SU(3) Haar measure. It is shown that this method is able to reproduce the available quantum lattice chromodynamics (QCD) data.

The canonically averaged quantum operator time correlation functions and related kinetic coefficients are calculated according to the Kubo formulas. In this approach CPIMC is used not only for calculation thermodynamic functions but also to generate initial conditions (equilibrium spatial, momentum, spin, flavor and color quasiparticle configurations) for generation the color phase space trajectories being the solutions of related differential dynamic equations. Correlation functions and kinetic coefficients are calculated as averages of Weyl's symbols of dynamic operators along these trajectories. Using this approach we have calculated the diffusion coefficient and shear viscosity, which not bad agree with experimental data obtained at RIHC.

*vladimir_filinov@mail.ru

Dielectric Response in Extreme Conditions Using Time-Dependent Density Functional Theory

A.D. Baczewski*, L. Shulenburger, M.P. Desjarlais, and R.J. Magyar
Sandia National Laboratories
Albuquerque, NM 87123, U.S.A.

Time-dependent density functional theory (TDDFT) is a powerful framework for solving the dynamical quantum many-electron problem. It is theoretically exact but requires the development of non-perturbative approximations in practice[1]. In conjunction with Ehrenfest dynamics TDDFT provides access to a wide variety of many-body response functions of experimental relevance through a direct calculation of real-time electron-ion dynamics. We have developed an Ehrenfest-TDDFT capability for studying the dielectric response of extended warm dense systems using the Projector Augmented Wave (PAW) method[2] that is numerically accurate, stable, and scalable. We will discuss the use of this new tool for calculations ranging from electronic stopping power and optical response to the dynamic structure factor, a quantity of fundamental importance to burgeoning X-Ray Thomson Scattering (XRTS) experimental capabilities. Focus will be placed upon both the computational advantages of this framework, as well its theoretical strengths and open questions concerning its foundations at elevated temperature.

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Security Administration under contract DE-AC04-94AL85000.
*adbacze@sandia.gov

[1] C. Ullrich. *Time-dependent density-functional theory: concepts and applications.* Oxford University Press, 1st Ed., (2011).

[2] G. Kresse and D. Joubert. *From ultrasoft pseudopotentials to the projector augmented-wave method.* Physical Review B, **59** 1758, (1999).

Ionization potential depression in hot dense plasmas through a pure classical model

A. Calisti*, S. Ferri and B. Talin
Aix Marseille Université, CNRS, PIIM UMR 7345
13397, Marseille, France

It is well known that the ionization potential of an ion imbedded in a plasma is lowered due to the whole charged particles (ions and electrons) interacting with that ion. It is the so called plasma effect. The numerical plasma model developed years ago[1,2], based on classical molecular dynamics, capable to describe a neutral plasma at equilibrium involving ions of various charge states of the same atom together with electrons, is used to investigate the ionization potential depression (IPD). The behavior of ionic species is controlled by a mechanism of collisional ionization-recombination mediated by the electrons. As usual in MD techniques, physical quantities are accessible by statistical sampling. The model relies on a limited set of postulates. The ion-electron interaction potential depends on the ionic species. For each one, the electron-ion potential is regularized (finite at short distance) and its minimum magnitude matches the ionization potential of the corresponding un-perturbed ion species. Both the ion-ion and the electron-electron potentials are Coulomb potentials at short distances. For an ion, the ionization-recombination process is ruled by the total energy of the two nearest neighbor electrons. Depending on the sign of their total energy, electrons are defined either as excited, i. e., trapped by an ion, or free. In order to compensate small gain or loss of energy during ionization or recombination events, the model requires limited temperature adjustments of the free electron population. The model does not require any further approximation, it results very robust, flexible and rather fast for providing the whole static and dynamics properties useful for laboratory laser plasma studies.
The study of the IPD is illustrated and discussed for aluminum plasmas at solid density and electron temperature varying from 70eV to 190eV. An equivalent study is carried out for cases of warm-dense beryllium ignoring partial electron degeneracy. The method relies on a sampling of the total potential energy of the electron located at an ion being ionized. The potential energy of such an electron results from the whole interacting charged particles interacting with it.
*annette.calisti@univ-amu.fr

[1] A. Calisti, S. Ferri, B. Talin, High Energy Density Physics, 5, 307 (2009).

[2] A. Calisti, B. Talin, Contrib. Plasma Phys. 51, 6, 524-528 (2011)

The calculation of diffusion coefficients in warm and hot dense matter

D. Saumon, C.E. Starrett and J.O. Daligault
Los Alamos National Laboratory
Los Alamos, NM 87545, U.S.A.

We have developed a model for warm and hot dense matter that couples an average atom model to describe electronic states with the theory of integral fluid equations for the ion correlations, using the quantum Ornstein-Zernike equations. Given an element, temperature and density, the model provides all electronic levels and wave functions, the interaction potentials, the average ion charge, and all correlation functions without any adjustable parameters. The electrons can be described quantum mechanically (Schroedinger equation) or semi-classically with the Thomas-Fermi model. The model has been successfully applied to the calculation of the ion-ion pair distribution function of elements from hydrogen to tungsten in the warm and hot dense matter regimes. We find very good agreement with quantum and Thomas-Fermi molecular dynamics simulations.
A more sensitive test of the ion-ion pair potential calculated within the model is the calculation of the ionic diffusion coefficient. While the model is intrinsically static, it provides self-consistently the ion-ion pair potential which can be used in a classical molecular dynamic simulation to calculate the diffusion coefficient. We will present an overview of the model and calculations of the diffusion coefficient for a range of materials and conditions. A comparison with the results of Thomas-Fermi molecular dynamics shows that this approach is remarkably efficient and accurate. The modeling of transport processes in white dwarf stars will benefit from this work.
*dsaumon@lanl.gov

Nuclear quantum effects on the structure and dynamics of dense hydrogen

Dongdong Kang[+], Jiayu Dai, Huayang Sun, and Jianmin Yuan*
Department of Physics, National University of Defense Technology,
Changsha, Hunan 410073, P. R. China

Due to its low mass, hydrogen is expected to exhibit significant quantum effects, such as quantum delocalization, zero-point motion and quantum tunneling, especially under low temperatures and high pressures[1-3]. In order to have deep insight into these quantum effects in dense hydrogen, we investigate the structure and dynamical properties of dense hydrogen at densities up to 100 g/cm^3 with the temperature range of 0.1-1 eV using first-principle path-integral molecular dynamics (PIMD)[4-6] simulations based on density functional theory. The simulation results show that quantum nature of nuclei has a significant effect on the structure and thermodynamic properties. Most importantly, the quantum dynamics such as scattering determined ionic diffusion, electrical conductivity, and thermal conductivity could be largely different from the classical results using the improved path-integral centroid molecular dynamics[7]. These results indicate that when the thermal de Broglie wavelength of nuclei is comparable with average interparticle distance, the nuclear quantum effects are not negligible even at high temperatures and give new results of structure and dynamical properties of dense matter under extreme conditions.

[+]ddkang@nudt.edu.cn
*jmyuan@nudt.edu.cn

[1] H. Kitamura, S. Tsuneyuki, T. Ogitsu, and T. Miyake, Nature 404, 259 (2000).
[2] J. A. Morrone and R. Car, Phys. Rev. Lett. 101, 017801 (2008).
[3] G. Geneste, M. Torrent, F. Bottin and P. Loubeyre, Phys. Rev. Lett. 109, 155303 (2012)
[4] D. Marx and M. Parrinello, J. Chem. Phys. 104, 4077 (1996).
[5] M. E. Tuckerman, D. Marx, M. L. Klein, and M. Parrinello, J. Chem. Phys. 104, 5579 (1996).
[6] D. Marx, M. E. Tuckerman, G. J. Martyna, Comput. Phys. Commun. 118, 166 (1999).
[7] D. Kang et al. submitted.

Solidification and Screening Enhancement in Asymmetric Binary Ionic Mixtures

H. D. Whitley,* W. E. Alley, J. I. Castor, A. Szöke, J. Nilsen, and H. E. DeWitt
Lawrence Livermore National Laboratory
Livermore, CA 94551, U.S.A.

The equation of state of binary ionic mixtures of similar ions, such as nitrogen, oxygen and carbon, has been extensively studied. The study of dense asymmetric mixtures, where $Z_2 >> Z_1$ and $m_2 >> m_1$, has primarily focused on mixtures of hydrogen and iron at solar conditions. Using molecular dynamics simulations, we examine the behavior of highly asymmetric binary ionic mixtures, where the coupling of the high-Z species may be orders of magnitude higher than the coupling of the low-Z species. For the conditions we have studied, we find that solidification occurs in the high-Z species, while the low-Z species exists as a freely flowing fluid within the high-Z solid matrix. Using the Widom expansion method, we compute the plasma screening enhancement of the nuclear reaction rates for $Z = 1$ in a high-Z matrix. Prepared by LLNL under Contract DE-AC52-07NA27344. LLNL-ABS-653077

*heather@llnl.gov

Temperature-dependent interatomic potential based on ab initio simulation

Huayang Sun, Jiayu Dai*, Dongdong Kang, Jiaolong Zeng and Jianmin Yuan
Department of Physics, National University of Defense Technology
Changsha, Hunan 410073, P. R. China.

Combining molecular dynamics, ab initio molecular dynamics is capable of simulating various dynamic behaviors relevant to temperatures, pressures and laser fields. However, because of the computational cost and limitation by parallel methods, AIMD is usually applied to systems containing a few hundreds of atoms, which condemns its application to the study of dynamic compression, phase transition, and transport behaviors. Although classical molecular dynamics can investigate large systems of more than 106 atoms, it requires accurate and wide range temperature-dependent interatomic potentials which are seldom available, in particular for the dense matter. Here, we construct new temperature-dependent interatomic potentials using neural network method, based on the structures and energies from AIMD using tens of atoms. The new potential is implemented in CMD and the computational efficiency is found improved by 103 times. Using the new potential, the calculated energies, pressures and melting points in a wide range of temperature and pressure are almost the same as that from the AIMD method. Based on this new approach, it is possible to investigate dynamic compression processes and phase transitions within the accuracy of ab initio method.

*jydai@nudt.edu.cn,
jydai203@163.com

DFT calculation of plasma frequency and free electron density in dense xenon plasma

I.M. Saitov

Joint Institute for High Temperatures
Russian Academy of Sciences
Moscow 125412, Russia

The reflectivity of shocked xenon was measured in the experiments of Mintsev and Zaporoghets in 1989 for wavelength $\lambda = 1064\,\text{nm}$ [1] and further for $\lambda = 694\,\text{nm}$ and $\lambda = 532\,\text{nm}$ [2]. But there is no adequete theoretical explanation of these reflectivity results in frames of the standard methods of nonideal plasma theory. As it was shown in [3, 4], the Drude model, with collisional frequency in Born approximation, gives reflectivities that are 2.5 – 3 times larger than the measured values at low densities. The results of other approaches to the collision frequency calculation also can't provide better explanation of steep slope of reflectivity drop with decreasing of density. As it was shown in [3, 4] the assumption of significant width to the shock front gives a good agreement with the experimental data. However, there are no evidences of this effect in experiment. It should be noted that the main goal of experiments [1,2] was estimation of free electron density and plasma frequency in shocked xenon. The absence of adequate theoretical explanation of the experimental results [1, 2] did not allow obtaining reasonable estimation for these parameters. In this work we use metod of estimation of plasma freqency, which is based on DFT calculation of dielectric fuction and reflectivity from shoked xenon. The imaginary part of the dielectric function is evaluated using the longitudinal expression for dielectric tensor. The real part is obtained by the Kramers-Kronig transformation. Quantum molecular dynamics simulation and VASP are used as in [5]. However as opposed to Desjarlais, some improvement of the formalism is introduced. The better agreement with the results for the wavelength 1064 nm [1] is obtained for both absolute values and density dependence. No arbitrary width correction of the energy gap between bound and free states like in [5] is made. Contrary to [3, 4] it is assumed in all the calculations, as in [5], that the shockwave front has no width, what is similar to the experimental conditions.

1. V.B.Mintsev, Yu.B.Zaporogets. Contrib. Plasma Phys. **29**, 493 (1989).
2. Yu.B.Zaporoghets, V.B.Mintsev, V.K.Gryaznov, V.E.Fortov, H.Reinholz, T.Raitza, G.Röpke. J. Phys. A: Math. Gen. **39**, 4329 (2006).
3. H.Reinholz, G.Röpke, I.Morozov, V.Mintsev, Yu.Zaporoghets, V.Fortov, A.Wierling. J. Phys. A: Math. Gen. **36**, 5991 (2003).
4. H.Reinholz, Yu.Zaporoghets, V.Mintsev, V.Fortov, I.Morozov, G.Röpke. Phys. Rev. E **68**, 036403 (2003).
5. M.P.Desjarlais. Contrib. Plasma Phys. **45**, 300 (2005).

Quantum Statistical Potentials for Electron-Ion Plasmas in the Random-Phase Approximation

In Gee Kim[†,1,2] and Michael S. Murillo[§,1,3]
[1]New Mexico Consortium, Los Alamos, NM 87544, U.S.A.
[2]University of New Mexico, Albuquerque, NM 87131, U.S.A.
[3]Los Alamos National Laboratory, NM 87545, U.S.A.

The electronic structure of warm-to-hot dense plasmas can be computed with a variety of techniques. Historically, quantum statistical potentials (QSPs) [1] have been employed in both molecular dynamics (MD) and integral equation (e.g., hypernetted chain) settings. QSPs have the distinct advantage that, while approximate, electron dynamics can be represented in MD settings [2,3]. QSPs are most often formulated through a two step process that includes computing a diffraction-corrected Coulomb pair interaction and a pair potential that incorporates the Pauli exclusion principle. Most QSPs in wide use are *not* density dependent and little is known about their accuracy [1,3]. Recently, however, modern versions of QSPs have been developed in the context of density functional theories [4,5]. Motivated by density functional theory we develop a new variant of QSPs in that we require the QSPs to exactly produce the density and pair-correlation functions for a two-component electron-ion plasma with arbitrary degeneracy in the random phase approximation (RPA). This condition leads to a set of non-linear matrix equations for the three interactions $u_{\rm ee}(r)$, $u_{\rm ei}(r)$, and $u_{\rm ii}(r)$, all of which are explicitly density dependent and non-linearly related, *i.e.*, diffraction and Pauli are inseparable. In such a formulation the new QSPs are obtained for the homogeneous electron gas; we require that the structure factors $S_{st}^{RPA}(q)$ $(s,t = {\rm e},{\rm i})$ of the interacting quantum system are represented by a classical system with the QSPs we seek. We perform a numerical quadrature for integrating the frequency of the dynamic structure factors $S_{st}^{RPA}(q,\omega)$ described in the fluctuation-dissipation theorem in terms of density-dependent finite-temperature Lindhard functions. Because of this numerical step, we provide a useful fit to our numerical results. The corresponding physical properties of two-component plasmas are discussed in detail and compared with those of older QSP formulations.

[1] C. S. Jones and M. S. Murillo, High Energy Density Phys. **2**, 379 (2007).
[2] J. N. Glosli *et al.*, Phys. Rev. E **78**, 025401(R) (2008)
[3] F. R. Graziani *et al.*, High Energy Density Phys. **8**, 105 (2012).
[4] M. W. C. Dharma-wardana and F. Perrot, Phys. Rev. Lett. **84**, 959 (2000).
[5] J. Dufty and S. Dutta, Phys. Rev. E **87**, 032101 (2013); S. Dutta and J. Dufty, *ibid.* **87**, 032102 (2013).

[†]igkim@newmexicoconsortium.org
[§]murillo@lanl.gov

A step towards a kinetic theory of strongly coupled Coulomb systems.

Jérôme Daligault
Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545

We present a systematic approach to develop renormalized kinetic equations that can describe the dynamics of classical, strongly-coupled fluids, including liquids and plasmas. Correlated interactions among particles are described by an effective (renormalized) potential that integrates the average effects of the fluid on the bare interactions. The basis of the theory is an effective action functional Ω of external potentials ϕ that contains all information about the dynamical properties of the system. In particular, its functional derivatives generate successively the single-particle phase-space density f and all the correlation and density response functions, which are coupled through an infinite hierarchy of evolution equations. Traditional renormalization techniques are then used to perform the closure of the hierarchy through memory functions. The memory functions satisfy a relation that can be used to devise systematic renormalized perturbative approximations in powers of the bare interparticle interaction. The present formulation can be equally regarded as (i) a generalization to dynamical problems of the density functional theory of fluids in equilibrium and (ii) as the classical mechanical counterpart of the theory of non-equilibrium Green's functions in quantum field theory. It unifies and encompasses previous results for classical Hamiltonian systems with any initial conditions. For equilibrium states, the theory reduces to the equilibrium memory function approach used in the kinetic theory of fluids in thermal equilibrium. For non-equilibrium fluids, popular closures of the BBGKY hierarchy (e.g. Landau, Boltzmann, Lenard-Balescu-Guernsey) are simply recovered. Important topical applications include the generalization of the Boltzmann equation to dense gases and liquids, and the kinetic theory of strongly coupled plasmas.
*daligaul@lanl.gov

[1] J. Daligault. *Renormalized Kinetic Theory of Classical Fluids in and out of Equilibrium* Journal of Statistical Physics **143**, 1189 (2011).

Influence of dynamic screening on the scattering cross sections of the particles of the dense semiclassical plasma

K.N. Dzhumagulova, E.O. Shalenov(*) , T.S. Ramazanov
IETP, al-Farabi Kazakh National University, Al-Farabi 71,
Almaty 050040, Kazakhstan

In work[1] the effective potential for electron – charge interaction considering both effects of screening and diffraction in the dense semiclassical plasma was presented. The way taking into account of the dynamic screening was proposed in work [2], where the static Debye radius was replaced by the dynamic screening radius:

$$r_o = r_D(1+\frac{v^2}{v_{Th}^2})^{1/2}. \quad (1)$$

Here v is the relative velocity of the colliding particles, v_{Th} is the thermal velocity of the particles in the system. Then the potential from [1] with dynamic screening can be rewritten as [3]:

$$\Phi_{\alpha\beta}(r) = \frac{Z_\alpha Z_\beta e^2}{\sqrt{1-4\lambda_{\alpha\beta}^2/(r_D^2(1+\delta^2))}}\left(\frac{e^{-Br}}{r}-\frac{e^{-Ar}}{r}\right), \quad (2)$$

where $A^2 = \frac{1}{2D^2}\left(1+\sqrt{1-4D_{\alpha\beta}^2/(r_D^2(1+\delta^2))}\right)$; $B^2 = \frac{1}{2D^2}\left(1-\sqrt{1-4D_{\alpha\beta}^2/(r_D^2(1+\delta^2))}\right)$;

$\delta = v/v_{Th}$ is the parameter of the relative velocity of the colliding particles.

In the same way the potential for electron-atom [4] taking into account the effect diffraction and dynamic screening effects has the following form:

$$\Phi_{ea}^{dyn}(r) = -\frac{e^2\alpha}{2r^4(1-4D_{ea}^2/r_o^2)}\left(e^{-Br}(1+Br)-e^{-Ar}(1+Ar)\right)^2, \quad (3)$$

where, $A^2 = \frac{1}{2D_{ea}^2}\left(1+\sqrt{1-4D_{ea}^2/r_o^2}\right)$, $B^2 = \frac{1}{2D_{ea}^2}\left(1-\sqrt{1-4D_{ea}^2/r_o^2}\right)$, $r_o = r_D(1+\frac{v^2}{v_{Th}^2})^{1/2}$.

Based on the new dynamic interactions models the scattering cross-sections of the plasma particles were investigated. Quantum mechanical method of phase functions was used for their calculation.

(*) shalenov.erik@mail.ru

[1] Ramazanov T.S., Dzhumagulova K.N. Effective screened potentials of strongly coupled semiclassical plasma. *Physics of Plasmas*. 2002.-Vol. 9.- P.3758-3761

[2] Kremp D., Schalges M., Kraeft W.-D. *Quantum Statistics of Nonideal Plasmas*, Berlin, Springer, 2005. - 326 p.

[3] K.N. Dzhumagulova, G.L. Gabdullina, E.O. Shalenov. Dynamic interaction potential and the scattering cross sections of the semiclassical plasma particles. *Physics of Plasmas*. - 2013. –Vol. 20. – P. 042702.

[4] Ramazanov T.S., Dzhumagulova K.N. and Omarbakiyeva Y.A. Effective polarization interaction potential "charge-atom" for partially ionized dense plasma. *Physics of Plasmas*. 2005. – Vol.12.- P.092702.

Impact of Screening and Ionization on Coulomb Coupling in Strongly Coupled Plasmas

L. G. Stanton[1,*] and M. S. Murillo[2]
[1]Lawrence Livermore National Laboratory, Livermore, CA 94551, U.S.A.
[2]Los Alamos National Laboratory, Los Alamos, NM 87545, U.S.A.

Coulomb coupling is traditionally defined by the parameter $\Gamma = Q^2/aT$, which is the ratio of a potential energy Q^2/aT (Q is the charge and a is the spacing) to a kinetic energy T (T is the temperature in energy units). We examine regimes of strong coupling in dense plasma experiments using a refined definition in which we compute the potential and kinetic energies directly from their thermodynamic definition and include the effects of finite ionization [1] and screening [2], which have recently been shown to have important impacts on coupling. We propose optimal experimental regimes that can be probed with XRTS to examine directly the physics of strong coupling.

*liam@llnl.gov

[1]M. S. Murillo *et al.* PRE **87**, 063113 (2013).
[2]M. Lyon, S. D. Bergeson, and M. S. Murillo PRE **87**, 033101 (2013).

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. LLNL-ABS-653176

THERMODYNAMIC PROPERTIES OF SEMICLASSICAL PARTIALLY IONIZED HYDROGEN AND HELIUM PLASMAS

M.T. Gabdullin*, T.S.Ramazanov, T.N. Ismagambetova, G.B. Ahtanova
[1]Al Farabi Kazakh National University, NNLOT, ITEP,
71, Al-Farabi av., Almaty, 050040, Kazakhstan

In this work the thermodynamic properties of partially ionized hydrogen and helium plasma were investigated, which consisting of electrons, ions and atoms for following parameters of temperature and number density: $n = 10^{20} \div 10^{24} cm^{-3}$ and $T = 10^4 \div 10^6 K$. Interactions between ionized particles were considered on the basis of the micropotential [1], which takes into account quantum-mechanical effects of diffraction and symmetry at small distances:

$$\varphi_{\alpha\beta}(r) = \frac{Ze_\alpha e_\beta}{r}\left(1-\tanh\left(\sqrt{2}\,\frac{\lambda_{\alpha\beta}^2}{a^2+br^2}\right)e^{-\tanh\left(\sqrt{2}\frac{\lambda_{\alpha\beta}^2}{(a^2+br^2)}\right)}\right)$$
$$\left(1-e^{-r/\lambda_{\alpha\beta}}\right)-\delta_{\alpha e}\delta_{\beta e}k_B T\ln\left(1-\frac{1}{2}\exp\left(-\frac{r^2}{\lambda_{ee}^2}\right)\right), \quad (1)$$

where $\lambda_{\alpha\beta}$ is the thermal wave length, a is the average distance between particles, α, β are the sort of particles and b = 0.033. The first term in the right sight of the equation (1) is the diffraction term and the second one is responsible for the symmetry effects. For interaction between ions the effective potential was used, which obtained in work [2]. Polarizability of atoms was taken into account in effective potentials [3]. Composition of partially ionized plasma was calculated via the Saha equation, which takes into account the reduction of the ionization potential derived from the potential [1-3]. Thermodynamic properties of plasma (internal energy and equation of state) were obtained through radial distribution functions and interaction potentials between particles, where collective effects were taken into account by solution of the integral equation of the Ornstein-Zernike. The hyper netted chain approximation (HNC) was used. The obtained results were compared with the data of other authors.

gabdullin@physics.kz

[1] Zh.A. Moldabekov, T.S. Ramazanov, K.N. Dzhumagulova, 2012, *Contrib.Plasma Phys.* 52 3.
[2] T.S. Ramazanov, K.N. Dzhumagulova, M.T. Gabdulin, 2010, *Phys. Plasmas* 17 042703.
[3] T.S. Ramazanov, K.N. Dzhumagulova, Yu.A. Omarbakiyeva, *Phys. Plasm.* 12, 092702 (2005).

Electrostatic particle based modeling for simulation of strongly coupled plasmas

Mayur Jain*, John Verboncoeur and Andrew Christlieb
Michigan State University
East Lansing, MI 48823, U.S.A.

This work focuses on the development of new modeling and simulation tools for studying strongly coupled plasmas (SCP) which differ from traditional plasmas in that their potential energy is larger than kinetic energy. The standard quasi neutral plasma model does not account for two major effects in SCP: 1) Change in the permittivity for modeling electromagnetic waves. 2) Impact on relaxation of charged particles undergoing Coulomb collisions with weakly shielded long range interactions. These objectives require the development of: (i) Electrostatic particle based models based on Particle in cell (PIC) and Boundary integral Treecode (BIT) methods (ii) Electromagnetic particle based models based on PIC and new implicit particle methods based on treecodes (iii) Continuum models with long range correlations incorporated through fractional derivatives in time. BIT is a mesh free method offering advantages in simulating resolved SCP with boundary conditions, whereas resolved PIC necessitates a prohibitively fine mesh when including boundary conditions. A treecode algorithm reduces operation count from $O(N^2)$ to O(N log N). The particles are divided into a hierarchy of clusters and particle-particle interactions are replaced by particle-cluster interactions evaluated using multipole expansions. Treecodes using monopole approximations and a divide-and-conquer evaluation strategy have been very successful in particle simulations. With an ongoing interest in optimizing their performance, BIT is an ideal method for studying strongly coupled electrostatic plasmas consisting 10^8 atoms. In this context BIT can be used to simulate a one to one representation of the ultra cold SCP, each particle representing a physical particle, naturally resolving long range interactions. Current work includes studying oscillations and expansion in strongly coupled plasmas and electron and ion correlations in comparison with the existing work.

This project is supported by an AFOSR Basic Research Initiative on Ultra Cold Plasmas

*jainmayu@msu.edu
johnv@msu.edu
christli@msu.edu

[1] J.Barnes and P. Hut. A hierarchical O(nlogn) force-calculation algorithm. Nature 324,(1986)
[2] A.J. Christlieb, R. Krasny, J.P. Verboncoeur, J.W. Emhoff, and I.D. Boyd, Grid-free plasma simulation techniques, IEEE Transactions on Plasma Science 34 (2006).
[3] S. Kulin, TC Killian, SD Bergeson, and SL Rolston. Plasma oscillations and expansion of an ultracold neutral plasma. Physical Review Letters,
85(2):318–321, 2000.

Two-dimensional distribution of plasma parameters in the He/H_2 gas mixtures in a stratified glow discharge

Bastykova N.Kh., Kodanova S.K.*, Ramazanov T.S.
IETP, Al-Farabi Kazakh National University
71 Al-Farabi av., Almaty 050040, Kazakhstan

Striations associated with the rate of the atoms excitation by the electron impact can be formed in positive column (PC) of a glow discharge. Positive column of a glow discharge is widely used in the gas-discharge light sources, plasma chemistry and etc. Most contributions in describing of kinetic models of the glow discharge stratification were made in works [1-6]. Using a mixture of different gases in glow discharge leads to a very significant change in the characteristics of both the electron and ion components of the plasma [7-8]. In this work axial distribution of plasma parameters was calculated by solving the Boltzmann equation for the EEDF, the motion equations of the ions in the drift-diffusion approximation and the Poisson equation for the electric field distribution. The ambipolar diffusion approximation and the dependence of EEDF on electron total energy were used to obtain the radial distribution of plasma parameters. The positive column of a glow discharge in a mixture of He-H_2 gases at a value of pressure p = *0.5torr* and electric field E_0 = *3V/cm* was considered. Two-dimensional axial and radial distributions of the plasma parameters (electron density, electric field and electron temperature and etc.) in the positive column of discharge tube in helium at different number density of hydrogen impurity (0-10%) were obtained. It was shown that the addition of the hydrogen to helium significantly changes the characteristics of plasma discharge. The number of striations and electron density increase due to the lower ionization potential of hydrogen atom.

*kodanova@physics.kz

[1] I.B. Bernstein and T. Holstein *Phys. Rev.* 94 (1954) 1475
[2] L.D. Tsendin *Plasma Sources Sci. Technol.* 4 (1995) 200
[3] A.V. Fedoseev and G.I. Sukhinin *Plasma Phys. Rep.* 30 (2004) 1061
[4] V.I. Kolobov *J. Phys. D: Appl. Phys*. 39 (2006) R487–R506
[5] G.I. Sukhinin, T.S. Ramazanov, et.al. *J. Phys.D: Appl. Phys.*40 (2007) 407761.
[6] G.I. Sukhinin, A.V. Fedoseev, T.S. Ramazanov, et.al. *J.Phys. D: Appl. Phys.* 41 (2008) 245207.
[7] S.A. Maiorov, T.S. Ramazanov, K.N. Dzhumagulova, et.al. *Physics Of Plasmas* 15 (2008) 093701.
[8] T.S. Ramazanov, T.T. Daniyarov, S.A. Maiorov , et.al. *Contrib. Plasma Phys.*51(2011) 505 –508

Classical-map hypernetted chain calculations for multi-component plasmas

R. Bredow*, T. Bornath, W.-D. Kraeft, M.W.C. Dharma-wardana** and R. Redmer
Institut für Physik, Universität Rostock
Rostock, 18051, Germany.
**National Research Council of Canada
Ottawa, Canada.

Warm dense matter is of interest for modeling the interiors of planets and Brown Dwarfs. Corresponding pump-probe experiments are performed at free electron laser facilities such as FLASH, LCLS or the future XFEL in Hamburg. In this connection X-ray Thomson scattering is of special interest[1]. In order to explain or predict the X-ray Thomson scattering spectra simulations on the structural properties of plasmas are performed. While ab initio simulations are computationally expensive, semi-classical approaches can deliver fast results for pair distribution functions and static structure factors even for dense systems.

We solve the Ornstein-Zernike equation within the hypernetted chain (HNC) approximation for dense multi-component plasmas using the classical-map method[2]. This approach proposes to treat the quantum features of the electrons using an adapted temperature for the electron system while the ions are treated classically. Results for pair distribution functions and static structure factors are presented for dense hydrogen, beryllium, carbon and CH plasmas.

*richard.bredow@uni-rostock.de

[1] S.H. Glenzer and R. Redmer. *X-ray Thomson scattering in high energy density plasmas* Rev. Mod. Phys., **81**, 1625 (2009).

[2] M.W.C. Dharma-wardana and F. Perrot. *Simple Classical Mapping of the Spin-Polarized Quantum Electron Gas* Phys. Rev. Lett., **84**, 026401 (2000).

Variational Average-Atom in Quantum Plasma – review and recent progress

R. Piron*(1), T. Blenski(2), C. Caizergues(2), B. Cichocki(3)

(1) CEA, DAM, DIF, F-91297 Arpajon, France.
(2) CEA Saclay, IRAMIS, "Laboratoire Interactions Dynamique et Lasers", Centre d'Etudes de Saclay, F-91191 Gif-sur-Yvette Cedex, France.
(3) Institute of Theoretical Physics, Warsaw University, Hoza 69, 00-681 Warsaw, Poland.

The Variational Average-Atom in Quantum Plasma (VAAQP) code is based on a fully variational approach to atoms in plasmas [1,2], which can be viewed as a quantum extension of the well-known Thomas-Fermi (TF) model [3]. Contrary to other generalization of the TF model to quantum description of atoms in plasmas [4,5], the equations of the VAAQP model can be obtained from the minimization of an approximate free-energy and fulfills the virial theorem.

The practical implementation of the VAAQP approach was presented for the first time during the SCCS 2008 conference [6]. Since then, progress have been achieved as concerns the model and its applications. First, the numerical implementation has allowed us to check directly the thermodynamic consistency of the model [7]. It was also used to calculate dense plasmas equation-of-state in order to make comparisons with other approaches and experimental measurments of Hugoniot adiabats [8]. A particular attention was then paid to the virial theorem, which was derived in detail for both the non-relativistic and relativistic versions of the model, and numerically checked [8,9]. Later, a first application to the calculations of dense plasmas radiative properties was proposed [10], using a statistical approach [11] to an approximate Detailed Configuration Accounting version of the model. This very simple approach notably rely on the very common independent-particle approximation (see for example [12]). To go further this independent particle approach, work is in progress towards the calculation of radiative properties using a full self-consistent linear-response theory [13,14]. As a first step, the frequency-dependent linear-response of the Thomas-Fermi version of the model was carefully studied in the framework of Bloch's hydrodynamics [15].

* robin.piron@cea.fr

[1] R. P. Feynman, N. Metropolis, E. Teller, Phys. Rev. 75:1561 (1949)
[2] B. F. Rozsyai, Phys. Rev. A 5:1137 (1972)
[3] D. A. Liberman, Phys. Rev. B 20:4981 (1979)
[4] T. Blenski, B. Cichocki, Phys. Rev. E 75:056402 (2007)
[5] T. Blenski, B. Cichocki, High Energy Density Phys. 3:34 (2007)
[6] R. Piron, T. Blenski, B. Cichocki, J. Phys. A 42:214059 (2009)
[7] R. Piron, T. Blenski, B. Cichocki, High Energy Density Phys. 5:258 (2009)
[8] R. Piron, T. Blenski, Phys. Rev. E 83:026403 (2011)
[9] R. Piron, T. Blenski, High Energy Density Phys. 7:346 (2011)
[10] R. Piron, T. Blenski, High Energy Density Phys. 9:702 (2013)
[11] F. Perrot, Physica A 150:357 (1988)
[12] W. R. Johnson, C. Guet, G. F. Bertsch, J. Quant. Spect. Rad. Transf. 99:327 (2006)
[13] T. Blenski, J. Quant. Spect. Rad. Transf. 99:84 (2006)
[14] T. Blenski, R. Piron, C. Caizergues, B. Cichocki, High Energy Density Phys. 9:687 (2013)
[15] C. Caizergues, T. Blenski, R. Piron, High Energy Density Phys., page tbd (2014)

A Practical way to Extend Plasma Transport Theory to Strong Coupling

Scott D. Baalrud,[(a)]* Kim Rasmussen,[(b)] and Jérôme Daligault[(b)]

(a) Department of Physics and Astronomy, University of Iowa, Iowa City, IA 52242

(b) Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545

In this work, we describe a physically intuitive method for extending traditional plasma transport theories to strong coupling [1,2]. Like the traditional theories, ours is based on a binary collision picture. The extension to strong coupling is achieved by taking the interaction potential of binary scatterers to be an effective potential that includes many-body correlation effects. This effective potential is associated with the potential of mean force obtained by fixing the two scattering particles and averaging over the positions of all other particles. It is directly related to the pair distribution function [$g(r)$], which is well described by approximate theories from equilibrium statistical mechanics. In this work, we use the hypernetted chain (HNC) approximation to obtain an effective potential, but any other method could also be applied. The scattering cross section obtained from the effective potential provides the necessary input to the moment expansions of Chapman-Enskog or Grad. We have tested this approach by comparison with molecular dynamics simulations of self diffusion and viscosity of the one component plasma, as well as electron-ion temperature relaxation. We find that it is accurate up to the transition to liquid behavior that onsets as the coupling strength (Γ) approaches 50. For viscosity, it accurately models the kinetic contributions, but not the potential contributions that onset in the liquid regime. We also show that the accuracy of the theory can be improved by applying the effective potential to Enskog's kinetic equation for dense gases, rather than Boltzmann's kinetic equation for dilute gases. One advantage of the effective potential theory is that it can be incorporated into the hydrodynamics simulations used to model macroscopic behavior of complex systems, where a wide range of coupling strengths are often encountered. This is possible because it fits naturally within the Chapman-Enskog or Grad moment methods and because it is computationally efficient to evaluate.

*scott-baalrud@uiowa.edu

[1] S. D. Baalrud, and J. Daligault. *Effective Potential Theory for Transport Coefficients Across Coupling Regimes.* Physical Review Letters, **110**, 235001 (2013).

[2] S. D. Baalrud, and J. Daligault. *Extending Plasma Transport Theory to Strong Coupling Through the Concept of an Effective Interaction Potential.* Physics of Plasmas, in press (2014); arXiv:1403.1882v1.

On the origin of the surface term in the Ewald potential for periodic charged systems

V. Ballenegger*
Institut UTINAM, Université de Franche-Comté, UMR CNRS 6213, 25030 Besançon, France.

Molecular simulations are commonly performed under periodic boundary conditions and by using a lattice-sum method to solve the Poisson equation with the imposed periodicity, thereby avoiding any truncation of long-range Coulomb interactions [1]. The electrostatic potential at a point $\boldsymbol{r}$ in a simulation cell containing N particles j, with charge q_j and position $\boldsymbol{r}_j$, is then defined by the conditionally convergent lattice-sum

$$\Phi(\boldsymbol{r}) = \lim_{V\to\infty} \sum_{\boldsymbol{m}\in V} \sum_{j=1}^{N} \frac{q_j}{|\boldsymbol{r}-\boldsymbol{r}_j-\boldsymbol{m}|} \tag{1}$$

where $\boldsymbol{m}$ is a center of a periodic copy of the simulation cell. Due to distant coulomb interactions, the potential $\Phi(\boldsymbol{r})$ is sensitive, even in the limit $V\to\infty$, to the shape of the infinitely large periodic array of cells. As first shown by Redlack and Grindlay [2], $\Phi(\boldsymbol{r})$ can be decomposed in a purely periodic term, given by the Ewald formula [1], and a non-periodic term (extrinsic or surface contribution) that depends on the shape of V and on the total dipole and quadrupole moment of the simulation cell.
Several derivations of the Ewald formula that treat properly the conditionally convergent character of the lattice-sum (1) are available [3], but the surface term arises in these proofs from quite complicated calculations. We present a mathematically simple, and physically transparent, proof of the Ewald formula in which the surface term arises naturally from long-range contributions [4]. The discrepancy between different formulas obtained previously [5,6] for the surface contribution to the potential in a non-neutral simulation cell is furthermore resolved [4].

*vincent.ballenegger@univ-fcomte.fr

[1] D. Frenkel and B. Smit, *Understanding molecular simulation* (Academic Press, 1996)
[2] A. Redlack and J. Grindlay, J. Phys. Chem. Solids **36**, 73 (1975)
[3] S. Deleeuw, J. Perram, and E. Smith, Proc. R. Soc. Lond. A. **373**, 27 (1980); 373, 57 (1980); E. Smith, Proc. R. Soc. London, Ser. A **375**, 475 (1981); E. R. Smith, J. Chem. Phys. **128** (2008);
[4] V. Ballenegger, *On the origin of the surface term in the Ewald potential*, to appear in J. Chem. Phys. (2014)
[5] P. H. Hunenberger, in *Simulation and theory of electrostatic interactions in solution*, edited by L. R. Pratt and G. Hummer (AIP, New York, 1999) pp. 1783
[6] H. D. Herce, A. E. Garcia, and T. Darden, J. Chem. Phys. **126** (2007)

Dynamic collision frequency of Kelbg-pseudopotential-modelled plasmas

Yu.V. Arkhipov, A.B. Ashikbayeva, A. Askaruly*
Department of Physics and Technics, IETP, al-Farabi Kazakh National University,
Al-Farabi av. 71, Almaty 050040, Kazakhstan,
I.M. Tkachenko
Instituto de Matemática Pura y Aplicada, Universidad Politécnica de Valencia,
Camino de Vera s/n, 46022 Valencia, Spain

In the recent paper[1] a good agreement on the dynamic collision frequency has been achieved between the method of moments and the simulation data[2]. It is well established that the method of moments contains a free parameter function $Q(k,\omega)$, defined in the Nevanlinna function class, which has been obtained in the paper[1] on the basis of the known sum rules[3] and the asymptotic values[2] of the dynamic collision frequency.
In contrast to the above mentioned approach, there is an alternative way not to derive but to restore the Nevanlinna parameter-function. It essentially stems from the method of moments with local constraints[4], with an idea of construction dynamic characteristics using only three real nodes obtained from the simulation data.
In the present work the function $Q(k,\omega)$ is determined within the method of moments with local constraints applying two or three non-zero moments of the loss function defined by the imaginary part of the plasma inverse dielectric function[4] of the two-component plasma. It should be emphasized that within the two-moment approach the Nevanlinna parameter function is found as $Q(k,\omega)=i\nu(k,\omega)$, with $\nu(k,\omega)$ being the dynamic collision frequency which was introduced in the work[2] to take into account the spatial dispersion. On the other hand, the three-moment approach allows us to include collisional effects contained in the third moment[3] and, thus, to specify the dynamic collision frequency. Both approaches are used herein to reconstruct the Nevanlinna parameter-function and thus, to achieve a new insight in the application of the classical method of moments. The Nevanlinna parameter functions, derived in such a way, are consistent with all existing theories and can neatly be engaged to investigate the dynamic properties of strongly coupled Coulomb systems[5] in a wide range of plasma parameters.
*adilask@gmail.com

[1] Yu.V. Arkhipov, A.B. Ashikbayeva, A. Askaruly, A.E. Davletov, and I. M. Tkachenko. Optical Properties of Kelbg-Pseudopotential-Modelled Plasmas. *Contr. Plasma Phys.*, 53:375, 2013.

[2] I. Morozov, H. Reinholz, G. Röpke, A. Wierling, and G. Zwicknagel. Molecular dynamics simulations of optical conductivity of dense plasmas. *Phys. Rev. E,* 71:066408, 2005.

[3] Yu.V. Arkhipov, A. Askaruly, D. Ballester, A.E. Davletov, G.M. Meirkanova, and I.M. Tkachenko. Collective and static properties of model two-component plasmas. *Phys. Rev. E*, 76:026403, 2007.

[4] Yu.V. Arkhipov, A. Askaruly, A.E. Davletov, and I. M. Tkachenko. Dynamic Properties of One-Component Moderately Coupled. Plasmas: The Mixed Löwner-Nevanlinna-Pick Approach. *Contr. Plasma Phys.*, 50:69, 2013.

[5] I.M. Tkachenko, Yu.V. Arkhipov, A. Askaruly. *The Method of Moments and its Applications in Plasma Physics.* LAMBERT Academic Publishing, Saarbrücken, Germany, 2012.

Dynamically screened ion potential in the presence of streaming degenerate electrons

Zh. A. Moldabekov[1], P. Ludwig*[2], M. Bonitz[2], T. S. Ramazanov[1]
[1]Institute for Experimental and Theoretical Physics, Al-Farabi Kazakh National University, 050040 Almaty, Kazakhstan
[2]Institute for Theoretical Physics and Astrophysics, Christian Albrechts University Kiel, 24098 Kiel, Germany

The modeling of the dynamics of an electron-ion plasma is hampered by the large mass difference. We, therefeore, apply a multi-scale approach. It is based on a previously developed dynamical screening model that is extended to quantum systems at any degeneracy [1]. The scheme allows to accurately study the dynamics of strongly correlated classical ions in the presence of quantum degenerate, streaming electrons. In particular, this includes thermal and non-equilibrium electronic effects such as quantum wake effects, Friedel oscillations [2] and also electron magnetization.
In this contribution we present first results for the dynamically screened ion potential in linear response approximation in the presence of streaming electrons on the basis of (i) RPA, and (ii) the Mermin dielectric function where electronic collisions are included self-consistently [3,4].
The dependence of the characteristic oscillatory wake structure on the electron streaming velocity, electron degeneracy (temperature), and density is investigated. In particular, the transition from high temperature regime to low temperature regime is discussed. Strong deviations from the static Yukawa potential [5,6] as well as the possibility of an attraction between like-charged ions are shown.
*ludwig@theo-physik.uni-kiel.de

[1] P. Ludwig, M. Bonitz, H. Kählert, and J.W. Dufty, *Dynamics of strongly correlated ions in a partially ionized quantum plasma.* J. Phys.: Conf. Ser., **220**, 012003 (2010)
[2] D. Else, R. Kompaneets, and S. V. Vladimirov, *Shielding of a moving test charge in quantum plasma.* Phys. Rev. E, **82**, 026410 (2010)
[3] M. D. Barriga-Carrasco and A. Y. Potekhin, *Proton stopping in plasmas considering e^--e^- collisions.* Laser and Particle Beams, **24**,553 (2006)
[4] A. Y. Potekhin, D. A. Baiko, P. Haensel, and D.G. Yakovlev, *Transport properties of degenerate electrons in neutron star envelopes and white dwarf cores.* Astron. Astrophys., **346**, 345 (1999)
[5] T. S. Ramazanov, Zh. A. Moldabekov, M. T. Gabdullin, and T. N. Ismagambetova, *Interaction potentials and thermodynamic properties of two component semiclassical plasma.* Phys. Plasmas, **21**, 012706 (2014)
[6] T. S. Ramazanov, S. K. Kodanova, Zh. A. Moldabekov, and M. K. Issanova, *Dynamical properties of non-ideal plasma on the basis of effective potentials.* Phys. Plasmas, **20**, 112702 (2013)

SCCS 2014
Abstracts

Tuesday, July 29th

Towards dipolar quantum many-body physics with ultracold polar molecules

Silke Ospelkaus

Institut für Quantenoptik. Leibniz Universität Hannover
30173 Hannover, Germany

The long range dipolar interaction between polar molecules is expected to pave the way to the study of such intriguing phenomena as quantum magnetism, supersolids and novel anisotropic superfluids. In this talk, I will review recent experimental progress in the preparation, manipulation and control of polar molecules and their dipolar interactions. In particular, I will present experimental progress towards the preparation of ultracold ground state NaK molecules with a large dipole moment of about 2,7 Debye.

The Virial Theorem for Dirac Materials

Kevin S. Bedell[1] and James D. Stokes[1,2]

[1]Boston College, Chestnut Hill, MA USA
[2]Brookhaven National Laboratory, Upton, NY USA

The virial theorem in classical mechanics was first derived by Rudolf Clausius in 1870, [Phil. Mag. (1870)]. This has been applied to a variety of problems in classical and quantum mechanics. The theorem has been extended to quantum many-body problems and in particular to the d dimensional electron gas, dDEG. This has provided considerable insight into the role of interactions in the calculation of the ground state energy, E, in, for example, the 2DEG but it does not give an explicit result for E. We have recently derived the virial theorem for graphene and other Dirac materials for systems close to the Dirac point where the dispersion relation is linear. From this, we find for the d dimensional Dirac gas, dDDG, the exact form for the total energy is given by $E = B/r_s$ where $r_s a_0$ is the mean radius of the d-dimensional sphere containing one particle, with a_0 the Bohr radius, and B is a constant independent of r_s. This result implies that, given a linear dispersion and a Coulomb, 1/r, interaction, there is no Wigner crystallization in the dDDG, for d = 1, 2, or 3. It also follows that calculating B or measuring it at any value of r_s determines the energy, compressibility and other related thermodynamic quantities for all r_s. Our calculation of the compressibility for the 2DDG agrees with experiments done on graphene. We will describe the Fermi liquid theory for the 2DDG and 3DDG to make additional comparisons with experiment.

Phonons in two-temperature states of solid Aluminum and Gold

Louis Harbour[1]†, M. W. C. Dharma-wardana[2]*, Dennis Klug[2], and Laurent Lewis[1]
[1] Université de Montreal, Dept. de Physique, Montreal, Qc., Canada H3C 3J7
[2]National Research Council of Canada, Ottawa, On., Canada, K1A 0R6

Short-pulse lasers can be used to create and probe matter in various states where the ion subsystem temperature T_i is different from the electron-subsystem temperature T_e. We investigate the phonon-like ionic excitations of Aluminum and Gold, for given values of T_i, while T_e is varied, as would be the case when the laser-deposited energy is increased. While Al is a free-electron-like metal, Gold is a *d*-band metal. However, it turns out that a simple pseudopotential can be used for the class of problems studied here. The calculations are done using several methods (i) Using local pseudopotentials, and pair-potentials dependent on T_i, T_e, constructed according to Dharma-wardana et al [1-2], followed by a diagonalization of the dynamical matrix; (ii) using such pair-potentials in molecular-dynamics simulations using LAMMPS[3]; (iii) bench-marking the pair-potential calculations via *ab initio* simulations using the VASP[4] code and finite-temperature codes, where-ever this is feasible in an unambiguous, physically valid manner.
We expect to report on:
(a) equilibrium and two-temperature elastic constants and phonons for warm-dense solid Aluminum and Gold,
(b) the role of finite-T exchange and correlation in these calculations,
(c) information on lattice breakdown from the conversion of real phonon frequencies to complex frequencies.
(d) the validity or invalidity of the "phonon-hardening" hypothesis.
(e) The extent of the accuracy and applicability of the pair-potential approach which is numerically very simple and physically very transparent.
Preliminary results suggest that the 'phonon-hardening' hypothesis may not be applicable to warm-dense Al and Au solids.
†Louis.Harbour@umontreal.ca
*chandre.dharma-wardana@nrc-cnrc.gc.ca

1. M. W. C. Dharma-wardana, *Electron-ion and ion-ion potentials for modeling warm dense matter: Applications to laser-heated or shock-compressed Al and Si* Phys. Rev. E 86, 036407 (2012).
2. F. Perrot and M.W.C. Dharma-wardana, *Equation of State and electrical conductivity of mulitply ionized aluminum phases*, Phys. Rev. E. 52, no: 5 2920 (1995).
3. (LAMMPS) Large scale atomic molecular massively parallel simulator.
4. (VASP) Vienna ab-initio simulation package.

Consistency in transport calculations for strongly coupled plasmas

S.B. Hansen[1],* C.E. Starrett[2], D. Saumon[2], M. Desjarlais[1], A. Ng[3], and V. Recoules[4]
[1] *Sandia National Laboratories, Albuquerque, NM 87123, USA*
[2] *Los Alamos National Laboratory, Los Alamos, NM 87545, USA*
[3] *University of British Columbia, British Columbia V6T 1Z1, Canada*
[4] *CEA, DAM, DIF, F-91297 Arpajon, France*

The Ziman formulation is widely used to calculate electrical resistivities in liquid metals, warm dense matter, and high-temperature plasma. The calculated transport properties depend primarily on the static ion structure factor, the transport cross section, and the electron momentum distribution. In previous work [1], we have used ion structure factors from external models along with electronic quantities from an ion sphere model; here we explore the effects of enforcing consistency among these three quantities within a self-consistent average atom model [2] for H, Al, and Au and compare our results to those of Quantum Molecular Dynamics.

*sbhanse@sandia.gov
Sandia National Laboratories is a multiprogram laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under Contract No. DE-AC04-94AL85000.

[1] P.A. Sterne, S.B. Hansen, B.G. Wilson, and W.A. Isaacs, "Equation of state, occupation probabilities and conductivities in the average atom PURGATORIO code," *High Energy Density Physics* **3**, 278 (2007).

[2] C.E. Starrett and D. Saumon, "A simple method for determining the ionic structure of warm dense matter," *High Energy Density Physics* **10**, 35 (2014).

Pressure-driven Lifshitz Transition in 122-Pnictides

Khandker Quader*[1] and Michael Widom[2]
[1]Kent State University, Kent, OH 44242, U.S.A.
[2]Carnegie-Mellon University, Pittsburgh, PA 15206, U.S.A.

Strong underlying Coulomb interactions manifest themselves in striking properties of highly correlated condensed matter systems. Recently discovered iron-arsenic pnictides are one class of these systems. A substantive amount of work dealing with these strong Coulomb interactions are rooted in total energy density functional methods, while another large body of research employs different many-particle techniques on renormalized shorter-range interactions to ascertain emergent collective behavior. These often complement each other. In solids, specific space group symmetries related to the underlying periodic lattice also play important role.
The talk here pertain to work based on the first of the two complementary approaches that attempt to deal with Coulomb interactions in solids. Using first principles total energy calculations, we discuss that the observed pressure-driven anomalies in the 122-pnictides family (AFe_2As_2; A = alkali earth element Ca, Sr, Ba) can be understood as consequences of Lifshitz transitions arising from changes in Fermi surface topology at zero temperature. We also show that our results for energy band dispersions and spectra, lattice parameters, enthalpies, magnetism, and elastic constants over a wide range of hydrostatic pressure provide a coherent understanding of multiple transitions in these compounds, namely, enthalpic, magnetic and tetragonal (T) - collapsed tetragonal (cT) transitions. In particular, the T-cT transition and anomalies in lattice parameters and elastic properties, observed at finite temperatures, are interpreted as arising from proximity to T=0 Lifshitz transitions.
*quader@kent.edu

High pressure phase diagram for MgO

D. Cebulla* and R. Redmer
University of Rostock, Institute of Physics
18051 Rostock, Germany

The state of matter (e.g. temperatures and pressures) inside super-Earths, i.e., planets in the mass range 1-10 M_E, is much more extreme than in the interior of the Earth so that current experiments are not able to cover the whole density-temperature range directly [1]. In order to improve the understanding of the interior of exoplanets and their physical properties [2], *ab inito* calculations for the planetary materials are needed. A typical representative is MgO, which is an abundant material in the Earth's mantle. MgO is expected to be also important for the mantle of exoplanets as well as for the rocky cores of gas giants such as Jupiter [3].
Using *ab initio* molecular dynamic simulations (VASP [4]), we have determined the phase diagram for MgO up to 20000 K and 1.5 TPa. In particular, the transition from the solid to the molten salt has been studied using diffusion analyses and pair distribution functions. The transition from the NaCl- (B1) to the CsCl (B2) structure in solid MgO is determined by calculating the respective free enthalpies. The phase diagram of MgO is constructed based on the accurate equation of state (EOS) data. We compare with experimental results from (decaying) shock and ramp compression experiments [5, 6]. The B1-to-B2 and the liquid-solid transition line are compared with earlier simulation and experimental results [7].

*daniel.cebulla@uni-rostock.de

[1] D. Valencia, R.J. O'Connell and D. Sasselov, Icarus, **181**, 545 (2006)
[2] V. Stamenković, D. Breuer and T. Spohn, Icarus, **216**, 2 (2011)
[3] G. Kresse and J. Hafner, Physical Review B, **48**, 13115 (1993)
[4] F.H. Wilson and B. Militzer, Physical Review Letter, **108**, 111101 (2012)
[5] R.S. McWilliams, D.K. Spaulding, J.H. Eggert *et al.*, Science, **338**, 1330 (2012)
[6] F. Coppari, R.F. Smith, J.H. Eggert *et al.*, Nature Geoscience, **6**, 926 (2013)
[7] D. Cebulla and R. Redmer, Physical Review B, (2014), accepted

Plasma-Plasma and Liquid-Liquid First-Order Phase Transitions

G.E. Norman*, I.M. Saitov and V.V. Stegailov
Joint Institute for High Temperatures of Russian Academy of Sciences
Moscow, 125412, Russia.

Three liquid-liquid first-order phase transitions are discussed: Landau-Zeldovich dielectric-metal transition, 1943[1], Norman-Starostin plasma phase transition, 1968[2] and a semiconductor-metal transition, 1989[3]. The transition[1] is a hypothesis; it was attached to the liquid-vapor coexistence curve with a triple point below the conventional critical point. All the area near and below the critical point, above and below the coexistence curve was carefully studied for some substances since that time, in particular for cesium and mercury. The metal-nonmetal transition was observed and investigated. It turned out to be smooth. No indication to a phase transition has been found. The transition[2] was also a hypothetical one. The origin of the phase transition was derived from the van der Waals-like competition of the short-range quantum repulsion, long-range effective Coulomb attraction and temperature. The phase difference was related to different degrees of ionization. Finally some experimental evidences are obtained. Metallization of fluid H_2 was observed, resistivity decreases almost 4 orders of magnitude[4]. The measurements in shock waves[5] in D_2 demonstrated the 20% increase of density at Mbar pressure, just in the density range, where a sharp, 5 orders of magnitude, increase of electrical conductivity is observed. Pulsed-laser heating above the melting line of H_2 at static pressures is used in the Mbar pressure region[6]; the anomaly observed in the heating curve correlated with theoretical predictions for the plasma phase transition. The liquid-liquid Brazhkin et al transition[3] was observed experimentally in the melt. The phase difference was related to different conductivities and viscosities. The transition was attached to the liquid-solid coexistence curve with a triple point not far from the extremum point of the curve. The similar liquid-liquid-solid triple point is now suggested for D_2/H_2 melt[6]. It looks as if transitions[2,3] belong to one and the same transition. The first is attributed to partially ionized area around the critical point. Another one manifests itself in the vicinity of the triple point. Possibility of a lower critical point is pointed to. Similarity and difference between transitions[2,3] are analyzed. Uncertainty of the free electrons concept in the strongly coupled plasmas is emphasized. Density of electron states is discussed for both classical and quantum VASP cases. So called "gap" between free and bound states is considered. Conductivity and plasma frequency are calculated.

* genri.norman@gmail.com

[1] L.D. Landau, Y.B. Zeldovich. On the relation between the liquid and the gaseous states of metals. *Acta Physico-Chimica U.R.S.S.* 183:80, 1943.

[2] G.E. Norman, A.N. Starostin. Untenability of the classical description of nondegenerate dense plasma. *High Temperature*. 6:394, 1968.

[3] V.V. Brazhkin, R.N. Voloshin, and S.V. Popova. Semiconductor- metall transition in liquid Se. *JETP Lett.,* 50:424, 1990. Translation from *Pis'ma ZhETF* 50:92, 1989.

[4] S.T. Weir, A.C. Mitchell, and W.J. Nellis. Metallization of Fluid Molecular Hydrogen at 140 GPa (1.4 Mbar). *Phys. Rev. Lett*., 76:1860, 1996.

[5] V.E. Fortov et al, Phase Transition in a Strongly Nonideal Deuterium Plasma Generated by Quasi-Isentropical Compression at Megabar Pressures. *Phys. Rev. Lett*. 99:185001, 2007.

[6] V. Dzyabura, M. Zaghoo, and I.F. Silvera. Evidence of a liquid-liquid phase transition in hot dense hydrogen. *Proc Natl Acad Sci U S A*. 110:8040, 2013.

Molecular Mixtures of Relevance to Planetary Interiors

E. R. Meyer*, L. A. Collins, J. D. Kress, and C. Ticknor
Los Alamos National Laboratory
Los Alamos, NM 87544, U.S.A.

Many extra-solar planets are expected to have interiors similar to that of Neptune and Uranus. Yet, our knowledge of the inner workings of Neptune and Uranus is incomplete. Additionally, the compositions of these newly found planets will not be identical to either Neptune or Uranus. Therefore, rather than compute the EOS for each possible planetary interior, it behooves us to understand the general behavior of mixtures relevant to these interiors. We present the results of varying the concentration ratios in a mixture of Methane, Ammonia, and Water using quantum molecular dynamics simulations. We show the onset of a super-ionic phase of the mixtures occurs for all mixing ratios.
*meyere@lanl.gov

First-principles evaluation of the entropy of silicon dioxide and thermodynamics of giant impacts

Sebastien Hamel
Lawrence Livermore National Laboratory
Livermore, CA 94551, U.S.A.

Shock compression experiments provides us with a direct measurement of the equation of state of materials such as SiO_2 at the pressure and temperatures relevant to planetary science. The high-pressure response of materials to shock compression is cast in the form of a Hugoniot curve which is one of the key experimental inputs to equation of state models used in various hydrodynamic simulations of materials under extreme conditions of pressure and temperature. States on the principal Hugoniot also happen to be the collection of thermodynamic states reached during giant impacts between astrophysical bodies, including the one thought to be responsible for the formation of the Earth-Moon system [1,2]. The relevant pressure range for such impacts are in the hundreds of GPa, conditions that can be reached on several platforms such as the Omega Laser facility, NIF, the Z machine, and LCLS. The adiabatic expansion of the shocked material and its eventual partitioning into a vapor and/or a liquid phase is determined by the entropy reached during the shock compression. Entropy is a difficult quantity to extract from first-principles simulations and its accurate evaluation is one of the important recent development in electronic structure calculations. We present first-principles results for the entropy of silicon dioxide on the principal Hugoniot. The calculations are based on quantum molecular dynamics and thermodynamic integration using the coupling constant method. Comparisons are made to recent experimental results [3] and to several equation of state models.
*hamel2@llnl.gov

[1] M. Cuk, S.T. Stewart. *Making the Moon from a Fast-Spinning Earth: A Giant Impact Followed by Resonant Despinning* Science **338** pp. 1047-1052 (2012).

[2] R.M. Canup. *Forming a Moon with an Earth-like Composition via a Giant Impact* Science **338** pp. 1052-1055 (2012).

[3] R.G. Kraus, S.T. Stewart, D.C. Swift, C.A. Bolme, R.F. Smith, S. Hamel, B.D. Hammel, D.K. Spaulding, D.G. Hicks, J.H. Eggert and G.W. Collins. *Shock vaporization of silica and the thermodynamics of planetary impact events* J. Geophys. Res. **117** E09009 (2012).

Species Diffusion in Plasma Mixtures

Robert E. Rudd* and Tomorr Haxhimali
Lawrence Livermore National Laboratory
Livermore, CA 94551, U.S.A.

The diffusion of ions in a plasma is a non-equilibrium process that occurs in response to concentration gradients and other drivers. In weakly coupled plasmas the rate of diffusion is largely governed by binary collisions, and the diffusivity can be calculated reliably using Chapman-Enskog theory. As typical of this kind of calculation, the well-known result includes a Coulomb logarithm. When the plasma is more strongly coupled, the binary scattering approximation fails and the Coulomb logarithm becomes problematic. Here we report the results of another approach to diffusivity in plasma mixtures, an approach that continues to work when one or more of the components of a plasma mixture are strongly coupled and many-body scattering processes are important. The approach is to use classical molecular dynamics (MD) with an effective inter-ion potential. The potential accounts for electron screening without incurring the computational cost of explicit, dynamic electrons.

Specifically, this presentation will focus on two topics. The first is the nature of interdiffusion in an asymmetric plasma mixture in which one component (deuterium) is weakly coupled and the other component (argon) is strongly coupled. We use Green-Kubo techniques to calculate the self-diffusivities and the mutual diffusivity in the D-Ar mixture at 100 eV. We test the validity of proposed relations between the self-diffusivity and the interdiffusivity. We assess the importance of cage effects and long-time tails. We also examine how well the Chapman-Cowling model and other kinetic models describe the diffusion in the MD system.

The second topic is direct numerical simulation of the broadening of an interface between two species due to interdiffusion. Whereas the Green-Kubo calculations are done in an equilibrium MD simulation, the interface broadening is inherently non-equilibrium and requires a large-scale MD simulation. In this case we simulated 33 million ions. We compare the observed mutual diffusivity to the results from the Green-Kubo calculations, and analyze the mechanisms of diffusion.

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

*robert.rudd@llnl.gov

[1] T. Haxhimali and R. E. Rudd, "Diffusivity of Mixtures in Warm Dense Matter Regime," in *Frontiers and Challenges in Warm Dense Matter*, F. Graziani, M. Desjarlais, R. Redmer, and S. Trickey, eds. (Springer-Verlag, New York, 2014).

MD simulations and kinetic theory calculations of energy and particle transport processes in plasmas

L. X. Benedict*
Lawrence Livermore National Laboratory
Livermore, CA 94550, U.S.A.

Over the past 8+ years, the Cimarron group at LLNL has conducted an extensive set of simulations on electron-ion temperature equilibration, and electrical and thermal conductivities of plasmas using various quantum statistical potentials (QSPs). In this talk, I review what we have learned from these studies, paying particular attention to our efforts to understand the results using both classical and quantum kinetic theories of the Lenard-Balescu type. I hope to convey two main points: 1. QSPs, though chiefly intended for the simulation of static properties, are a useful tool for simulating dynamical properties as well, though it can be argued that certain QSP forms are more sensible to use than others, depending on the application. 2. The problems of plasma conduction, energy exchange, etc., for strongly-coupled oppositely-charged plasmas are still far from being considered solved problems.

*benedict5@llnl.gov

This work was performed under the auspices of the US Department of Energy by Lawrence Livermore National Laboratory under Contract No. DE-AC52-07NA27344.

Modelling fast electron transport in warm dense carbon

P. Mabey[1]*, N. J. Hartley[1], H. W. Doyle[1], C. R. D. Brown[1,2,3], A. P. L. Robinson[4] and G. Gregori[1]
[1]Department of Physics, University of Oxford,
Parks Road, Oxford OX1 3PU, UK
[2]AWE, Aldermaston
Reading, Berkshire RG7 4PR, UK
[3]Plasma Physics Group, Blackett Laboratory, Imperial College London,
Prince Consort Road, London SW7 2AZ, UK
[4]Central Laser Facility, Rutherford Appleton Laboratory,
Chilton, OX11 0QX, UK

It has recently been discovered that many white dwarf stars are primarily composed of carbon rather than hydrogen or helium as most theories would suggest[1]. The behaviour of carbon at very high temperatures and pressures is however poorly understood. It has been predicted that carbon crystallises to form a bcc lattice when the coupling parameter, Γ, becomes sufficiently large[2]. With the recent advances made in the field of high power lasers, such a state is now accessible in the laboratory. In this talk we outline a method of creating an off-Hugoniot strongly coupled carbon state using the Vulcan laser facility in the UK. The experimental conditions are simulated using fast electron transport models implemented in the Zephyros code.

*paul.mabey@physics.ox.ac.uk

[1] P. Dufour, J. Liebert, G. Fontaine & N. Behara, Nature, **450**, 522, (2007).

[2] S. Hamaguchi, R. T. Farouki & D. H. E. Dubin, Phys. Rev. E, **56**, 4671, (1997).

Toward Quantum Molecular Dynamics
Of The Electron Density with Classical Nuclei

Andreas Markmann[1] , Michael S. Murillo[2] , Victor S. Batista[1] , Frank Graziani[3]
[1] Yale University
New Haven, CT 06520, U.S.A.
[2] Los Alamos National Laboratory
Los Alamos, NM 87545, U.S.A.
[3] Lawrence Livermore National Laboratory
Livermore, CA 94551, U.S.A.

Treating electrons as classical particles in simulations of plasmas leads to unwanted and unphysical results that predict incorrect electromagnetic field interaction and collapse of electrons towards nuclei due to multiparticle collisions.

As a step toward consistent dynamics of the electron density with classical dynamics of the nuclei in a plasma, quantum dynamics of the six-dimensional Wigner density have been implemented. The method rests on the propagation of a transformed version of the Wigner density in phase space which allows the use of established quantum wave-packet propagation methods. An accurate reference method is demonstrated and efficiency gains using approximate propagation methods are discussed.

*andreas.markmann@yale.edu

Proper Finite-temperature Density Functionals and Their Computational Implementation

D. Charkraborty, J.W. Dufty, V.V. Karasiev, and S.B. Trickey*
Dept. of Physics, Univ. of Florida
Gainesville FL 32611, U.S.A.

Quantum effects and transient aggregation states in warm dense systems make treatment by plasma techniques problematic, hence ab initio molecular dynamics (AIMD) is the best computational approach at present. In AIMD, the ion-electron forces arise from Born-Oppenheimer electronic structure calculations (the BO potential surface). For reasons of computational feasibility, free-energy density functional theory is used to calculate the electronic free energy. This raises two problems: the accuracy of the required approximate exchange-correlation (XC) density functionals and the KS computational cost-scaling bottleneck (costs scale as the cube of the number of thermally occupied orbitals).

We report progress on both problems. First, more than thirty years after the ground-state local spin-density approximation (LSDA) XC functional was obtained from purely first-principles Monte Carlo data, we have produced the corresponding finite-temperature LSDA [1]. We will present results comparing its use with ground-state functionals which show the clear import of its intrinsic temperature dependence. Second, we will present new AIMD calculations using orbital free DFT (OF-DFT) and our recently developed, fully non-empirical non-interacting free-energy generalized-gradient approximation functional [2] . OF-DFT in principle provides the same quantum statistical mechanics as KS but with T-independent computational cost scaling which goes as the system volume. The AIMD calculations used our new Profess@QuantumEspresso interface; its structure and features will be sketched. This computational tool and the competitive functionals it incorporates open new opportunities for AIMD simulations of WDM and cold plasmas.

(Supported by US DoE Grant DE-SC0002139.)

*trickey@ufl.edu

[1] V.V. Karasiev, T. Sjostrom, J. Dufty, and S.B. Trickey, Phys. Rev. Lett. **112**, 076403 (2014).

[2]V.V. Karasiev, D.Chakraborty, O.A. Shukruto and S.B. Trickey, Phys. Rev. B **88**, 161108(R) (2013).

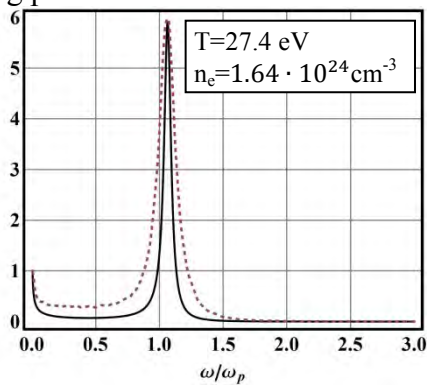
Dense plasma dynamic structure factor simulation data vs. the method of moments

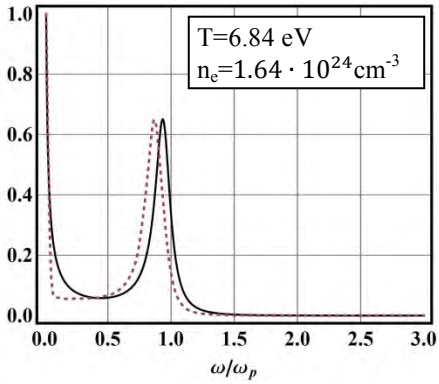
Yu.V. Arkhipov*, A.B. Ashikbayeva, A. Askaruly, A.E. Davletov, S. Syzganbaeva,
Department of Physics and Technics, IETP, al-Farabi Kazakh National University,
Al-Farabi av. 71, Almaty 050040, Kazakhstan,
I.M. Tkachenko
Instituto de Matemática Pura y Aplicada, Universidad Politécnica de Valencia,
Camino de Vera s/n, 46022 Valencia, Spain

Due to the difficulties of the experimental investigation of dense plasmas, numerical simulations have become an important tool of verification of theoretical approaches and vice versa. Here the simulation data[1] are compared to the results of the method-of-moments reconstruction of the "charge-charge" dynamic structure factor (DSF), $S(k,\omega)$, which is directly related to the plasma loss function $(-\mathrm{Im}\epsilon^{-1}(k,\omega)/\omega)$ via the fluctuation-dissipation theorem. The power moments of the loss function[2]: $C_l(k) = \int_{-\infty}^{\infty} \omega^{l-1}\left(-\mathrm{Im}\epsilon^{-1}(k,\omega)\right)\frac{\mathrm{d}\omega}{\pi}$: $C_0 = 1-\epsilon^{-1}(k,0)$, $C_2 = \omega_p^2$ and C_4 can be calculated in terms of the system partial static structure factors. The Nevanlinna theorem is applied to reconstruct the DSF normalized to its value at some frequency ω_0 close to zero:

$$\frac{S(k,\omega)}{S(k,\omega_0)} = \frac{\mathrm{Im}Q(k,\omega)}{\mathrm{Im}Q(k,\omega_0)}\left|\frac{\omega_0(\omega_0^2-\omega_2^2)+Q(k,\omega_0)(\omega_0^2-\omega_1^2)}{\omega(\omega^2-\omega_2^2)+Q(k,\omega)(\omega^2-\omega_1^2)}\right|^2, \qquad (1)$$

where ω_p is the plasma frequency, $\omega_1^2 = C_2/C_0$, $\omega_2^2 = C_4/C_2$; $Q(k,\ \omega)$ is the Nevanlinna parameter function (NPF). The simulations were carried out for three different effective potentials, particularly, the Deutsch potential, and we have calculated the two-component plasma partial structure factors by solving the Ornstein-Zernike equation in the hyper-netted approximation for these potentials. The NPF was determined to make the system dielectric function satisfy the Perel' - Eliashberg exact asymptotic form[2,3]. A satisfactory level of agreement was achieved with all data studied in the work[1], see e.g. the graphs, where we display the values of the function (1) calculated for the Deutsch effective potential and compared to the corresponding data[1] (dashed line), and where the Langmuir mode negative dispersion emerges as the coupling parameter increases.





*Yuriy.Arkhipov@kaznu.kz

[1] G. Zwicknagel, T. Pschiwul. Dynamic response of two-component model plasmas. *Contr. Plasma Phys.*, 43:393, 2003.

[2] I.M. Tkachenko, Yu.V. Arkhipov, A. Askaruly. *The Method of Moments and its Applications in Plasma Physics.* LAMBERT Academic Publishing, Saarbrücken, Germany, 2012.

[3] V.I. Perel', G. M. Eliashberg. Absorbtion of electromagnetic waves in a plasma. *Sov. Phys. JETP*, 14:633, 1962.

The Helmholtz Beamline at XFEL

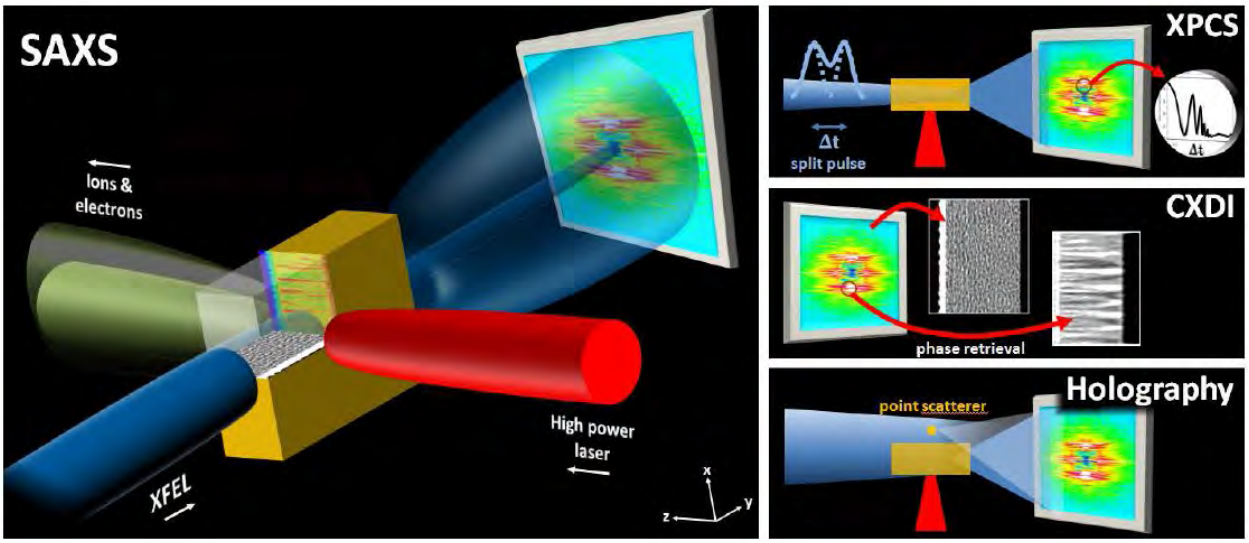
Probing solid density laser-plasma physics with XFELs on the femtosecond scale

M. Bussmann*, T. Kluge, L. Huang, T.E. Cowan
Helmholtz-Zentrum Dresden-Rossendorf
Bautzner Landstrasse 400, 01328 Dresden, Germany

We show that probing the ionization evolution and plasma dynamics in high power laser interaction with matter on the femtosecond and nanometer scale is in reach with state of the art X-ray lasers at facilities such as LCLS, SACLA and the European XFEL [1], where a facility that places a high power laser next to XFEL, the Helmholtz Beamline at XFEL, is planned.

We have conducted particle-in-cell simulations including radiative and collisional atomic processes to generate absolute predictions for synthetic scattering images using SAXS and RCXDI techniques. We could show that plasma dynamics from the target front side and bulk can be distinguished and plasma instabilities identified and their development could be temporarily involved.

Including atomic physics models from SCFly we could furthermore show that the temporal evolution of the ionization dynamics can be probed by resonant scattering.



Setup and synthetic scattering images for SAXS, XPCS, CXDI and Holography using a high power laser (shown in red) and an X-ray free electron laser (depicted in blue).

*m.bussmann@hzdr.de

[1] Kluge, T.; Gutt, C.; Huang, L.; Metzkes, J.; Schramm, U.; Bussmann, M.; Cowan, T. E., *Using XFELs for Probing of Complex Interaction Dynamics of Ultra-Intense Lasers with Solid Matter*, **Physics of Plasmas 21(2014), 033110**

Path Integral Monte Carlo calculations of internal partition functions for composite particles in quantum plasmas

D. Wendland[*,†,‡], A. Alastuey[†] and V. Ballenegger[‡]

[†] Laboratoire de Physique, ENS Lyon, 46 allée d'Italie, 69007 Lyon, France

[‡] Institut UTINAM, Université de Franche-Comté, 16 route de Gray, 25030 Besançon, France

The study of the thermodynamics of a quantum Coulomb system made with nuclei and electrons is motivated not only by its theoretical interest but also by a wide range of applications, especially in astrophysics where very precise equations of state (EOS) are needed, for instance in heliosismology.

Common chemical approaches assume preformed constituents and employ effective potentials and ad-hoc regularizations of divergent internal partition functions of the composite particles [1]. We aim instead for a first-principles description of the hydrogen-helium mixture made up of electrons, protons and α-nuclei interacting via the Coulomb potential, in a diluted but nevertheless strongly coupled low-temperature regime where a significant fraction of charges is bound into atoms, ions or molecules. Our approach is based on the screened cluster representation, which allows to treat all screening, recombination and interaction phenomena in a consistent way [2]. In a low-density and low-temperature regime, the scaled low temperature (SLT) expansion of the EOS has been derived for the pure hydrogen system, which rigorously extends the validity domain of the usual virial expansion into the partially or fully recombined atomic phase [3,4]. The SLT expansion of the EOS for pure hydrogen, and its extension to the hydrogen-helium mixture, involve temperature-dependent quantities, representing internal partition functions in the vacuum of the corresponding composite particles ($H^-, H_2^+, He, ...$). Those cluster partition functions are finite thanks to truncation inherited from screening.

We use the path integral representation and Monte Carlo techniques to compute numerically three-body partition functions. Efficient Monte Carlo sampling of those functions is achieved, even at quite low temperatures, thanks to the introduction of a simple importance sampling function that mimics the exact two-body density matrix [5]. An excellent agreement is found with the available analytic expressions for two-body clusters. We compare also our results with phenomenological partition functions for ions H^- and H_2^+ derived elsewhere [4].

*david.wendland@ens-lyon.fr

[1] D. Saumon et G. Chabrier, Phys. Rev. A **46**: 2084 (1992).
[2] A. Alastuey, V. Ballenegger, F. Cornu and P. A. Martin, J. Stat. Phys. **113**: 455-503 (2003)
[3] A. Alastuey, V. Ballenegger, F. Cornu, and P. A. Martin, J. Stat. Phys. **130**: 1119–1176 (2008).
[4] A. Alastuey and V. Ballenegger, Phys. Rev. E, **86**: 066402, 2012.
[5] D.Wendland, A. Alastuey and V. Ballenegger, submitted to Contributions to Plasma Physics (2014).

Kinetic Theory Molecular Dynamics and Hot Dense Matter

F. R. Graziani* and J. D. Bauer
Lawrence Livermore National Laboratory
Livermore, CA 94551, U.S.A.

M. S. Murillo
Los Alamos National Laboratory
Los Alamos, NM 87544, U.S.A.

Electrons are typically weakly coupled in hot, dense matter that is created in high-energy-density experiments. However, they are mildly quantum mechanical and the ions associated with them may be strongly coupled and classical. We develop a method that combines a Wigner kinetic treatment of the electrons with classical molecular dynamics for the ions. We refer to this hybrid method as "kinetic theory molecular dynamics," or KTMD. KTMD provides a framework for simulating plasmas in the hot, dense regime as current computational methods are generally limited by their inability to treat the dynamical quantum evolution of the electronic component. Using the N-body von Neumann equation for the electron-proton plasma, three variations of KTMD are obtained. The first approach yields a closed set of equations consisting of a mean-field quantum kinetic equation for the electron one-particle distribution function coupled to a classical Liouville equation for the protons. The latter equation includes both proton-proton Coulombic interactions and an effective electron-proton interaction that involves the convolution of the electron density with the electron-proton Coulomb potential. The mean-field approach is then extended to incorporate equilibrium electron-proton correlations through the Singwi-Tosi-Land-Sjolander (STLS) ansatz. The STLS contribution produces an effective electron-proton interaction that involves the electron- proton structure factor, thereby extending the usual mean-field theory. A third variation of KTMD is proposed by again extending the mean field approach. A set of coupled equations for the electron Wigner function and the electron-electron and electron-proton correlation functions are coupled to a classical Liouville equation for the protons. This latter variation has both time and momentum dependent correlations. In this way it is an improvement over STLS but it still requires that the correlations be weak.

*graziani1@llnl.gov

.

Nonlinear response theory of non-ideal charged and neutral matter

G.A. Pavlov*
Institute of Problems of Chemical Physics RAS,
Chernogolovka, Moscow region, 142432, Russia

The nonlinear response theory approaches are developed to study the nonlinear phenomena for charged dense matter and nonlinear transport in non-ideal charged and neutral systems.

The nonlinear phenomena: plasma wave echo and waves transformation have been investigated under non-ideal Coulomb system conditions based on a variant of the nonlinear response theory. Some general restrictions on the values of quadratic response functions are considered. The model for the determination of quadratic response functions is presented. The conditions for experimental realization of the mentioned phenomena in non-ideal plasma are examined. It is shown that ultra-short field pulses can induce the phenomena. Other nonlinear phenomena in non-ideal charged matter can be considered in the offered way. The studying of frequency moments and corresponding explicit approximations of response functions, described nonlinear phenomena, would be performed in these cases.

The theory of non-linear transport is elaborated to determine the Burnett kinetic coefficients of non-ideal multi-element matter. The Mori's algorithm is used to derive the equations of motion of dynamical value operators in the form of the generalized nonlinear Langevin equations (GNLE) for a non-ideal system. The procedure of the comparison of the phenomenological conservation equations of a continuous charged (and neutral) medium and GNLE for corresponding dynamical variables is used for the definition of Burnett coefficients. In consequence, the expressions of kinetic coefficients have been found through the long-wavelength and low frequency limits of correlation functions. These expressions of coefficients correspond to responses on second order thermal disturbances (temperature, mass velocity, etc). The method for calculation of Burnett kinetic coefficients is developed. This method is based on the investigations of long-wavelength limits of correlation functions which determine the coefficients. Corresponding kinetic equations are used for the determinations of long-wavelength limits of correlation functions. The calculations of coefficients have been provided for a model system. It is important also provide the calculation of Burnett kinetic coefficients of non-ideal matter by computer modeling to get a comparison of analytical and numerical approaches.

Thus the report shows the difference and similarity between the variants of non-linear response theory on mechanical and thermal disturbances: the description of nonlinear phenomena and nonlinear transport in non-ideal charged matter[1].

The properties of the matrix of coefficients at highest derivatives in the set of conservation equations in the linearized Burnett approximation are discussed to establish a link between the results of the Burnett coefficients investigations and hydrodynamic problems. For this purpose the traditional and Burnett models of heat and mass transfer were also considered in a two elements medium with spatial heat production which is proportional to concentration of one of the elements. Investigation of the models was provided using computational multi-parameter nonlinear analysis and analytical methods. Characteristics of thermal regimes of the models were studied and compared. The comparison shows quality difference between heat regimes of the models. Results of thermal regimes modeling can be used for example in modern energetic apparatuses development[2].

* E-mail: pavl4411@yandex.ru

[1]. Pavlov G.A. *On the theory of nonlinear response in a nonideal plasma* Technical Physics, V. 53, Issue 6, P. 697-706, 2008

[2]. Pavlov G.A. and Troshchiev Yu.V. *Heat regimes in a medium with non-linear transport processes and spatial heat production* Int. J. of Heat and Mass Transfer, V. 62, P.661–667, 2013

Molecular Dynamics Simulations of Warm Dense Carbon

H. D. Whitley[1],* D. M. Sanchez[1,2], S. Hamel[1], A. A. Correa[1], and L.X. Benedict[1]
[1]Lawrence Livermore National Laboratory
Livermore, CA 94551, U.S.A.
[2]University of California San Diego
La Jolla, CA 92093, U.S.A.

Recent quantum molecular dynamics (QMD) studies of carbon at temperatures between 9000K and 100000K show that the ionic contribution to the specific heat behaves in a manner that is inconsistent with the Cowan model, which has been widely used for the construction of high-temperature liquid EOS.[1] Using classical molecular dynamics simulations, we compute the ionic contribution to the specific heat of carbon using a variety of effective interaction potentials. We show that the linearly screened Coulomb potential (ie. the Yukawa model), which is commonly applied in studies of ionized matter, fails to reproduce the ion-ion correlation functions from the QMD simulations. Interaction potentials that are derived to match the solid and liquid phase properties of carbon produce behavior that is more consistent with what is seen in the QMD. Prepared by LLNL under Contract DE-AC52-07NA27344. LLNL-ABS-653206

*heather@llnl.gov

[1] R.M. More, K.H. Warren, D.A. Young, and G.B. Zimmerman, Phys. Fluids 31, 3059 (1988).

Self-Diffusion in Weakly-to-Strongly Coupled Yukawa Systems

J. V. Stern and M. S. Murillo*
Computational Physics and Methods Group
Los Alamos National Laboratory
Los Alamos, NM 87545, U.S.A.

We investigate self-diffusion in strongly coupled Yukawa systems over a wide range of parameters spanning the weakly to strongly coupled regimes. Molecular dynamics, with the standard Green-Kubo relation and mean squared displacement, are used to compute the diffusion coefficients. From these results we construct a new "dynamical phase diagram" for self-diffusion for this system. Hundreds of MD runs were performed to identify *five* distinct regions in the Γ-κ Yukawa phase diagram, three of which are shown in the figure below.

We also wish to model the types of diffusion to illuminate the properties in each regime. As such, we have explored several Langevin-type models. We find that the simple Ornstein-Uhlenbeck processes, originally developed to model Brownian motion, captures well the behavior in the weakly coupled regime (shown in green below). Generalized Langevin equations (with memory) are introduced, and we find that this class of models can model the collective behavior in the density of states (Fourier transform of the VACF).

Large angle scattering has been shown to be important in ICF plasmas [Turrell et al. PRL 112, 245002 (2014)]. From our results, we are able to invert the self-diffusion coefficient to obtain an effective Coulomb logarithm. However, from our analysis employing various Langevin models, we note that the effective Coulomb logarithm is not likely to be transferrable to other processes due to the fundamental Markovian assumption of Fokker-Planck approaches.

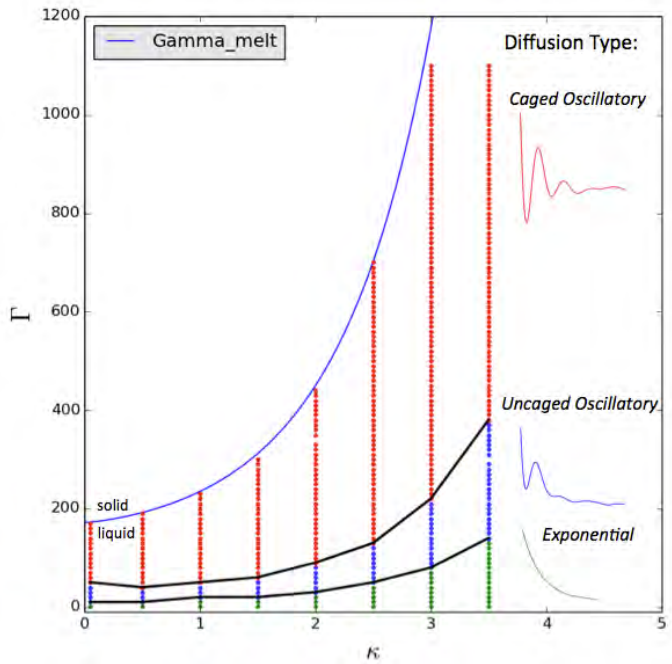


Figure 1: Phase diagram of VACF properties illustrating three of the types of diffusion: caged oscillatory (red), uncaged oscillatory (blue), and exponential decay (green). The VACF forms corresponding to the diffusion types appear on the right. Each point is a separate MD calculation.

*murillo@lanl.gov

Hierarchy of Static Fluctuation-Dissipation Theorems for the Classical One-Component Plasma

Kenneth I. Golden* and Joshuah T. Heath
Department of Mathematics and Statistics and Department of Physics
University of Vermont, Burlington, VT 05401-1455, U.S.A.

Fluctuation-dissipation theorems (FDTs) link transport coefficients (density response functions, e.g.) to n-point structure functions. The linear ($n = 2$) theorem has been a textbook example for a very long time [1]. The dynamical and static quadratic ($n = 3$) FDTs for the one-component plasma (OCP) were established some four decades ago [2]. Next came the static FDT linking the cubic response and four-point structure functions for the OCP [3]. We emphasize that the invariance of the three- and four-point structure functions under permutations of their wave vector arguments carries over into their companion quadratic and cubic response functions respectively in virtue of the FDTs; we refer to these invariance properties as "triangle" and "quadrangle" permutation symmetries.

In the present work, we derive the static quartic FDT for the OCP with the immediate goal of establishing a combinatorial formula representing the full FDT hierarchy. In this derivation, the system, which is always in a state of equilibrium, consists of a collection of N particles, each carrying charge Ze, pervaded by an external time-independent Coulomb potential. A straightforward statistical mechanical perturbation theoretic calculation then provides the Liouville distribution function to any order in the external potential. The average fourth-order density response, which is of interest here, is then calculated by ensemble averaging the microscopic density over the fourth-order distribution function. Comparison with the constitutive relation for the quartic density response function then yields the quartic FDT. Our result exhibits the expected pentangle permutation symmetry.

*Kenneth.Golden@uvm.edu

[1] H. Nyquist, *Physical Review* **32**, 110, 1928; H. B. Callen and T. A. Welton, *Physical Review* **83**, 34, 1951; R. Kubo, *Journal of the Physical Society of Japan* **12**, 570, 1957.

[2] K. I. Golden, G. Kalman, and M. B. Silevitch, *Journal of Statistical Physics,* **6** 87-118, 1972.

[3] K. I. Golden and G. Kalman, *Annals of Physics* **143**, 160-178, 1982.

.

A Gradient-Corrected, Analytic Screening Potential for Dense, Strongly-Coupled Plasmas

L. G. Stanton[1,*] and M. S. Murillo[2]

[1]Lawrence Livermore National Laboratory, Livermore, CA 94551, U.S.A.

[2]Los Alamos National Laboratory, Los Alamos, NM 87545, U.S.A.

We generalize the Yukawa potential to allow for moderate spatial variations in the electronic density and non-ideal contributions to the compressibility for both classical and quantum plasmas. Based on a gradient expansion around the Thomas-Fermi limit of density functional theory, the new potential contains a bifurcation that separates purely repulsive behavior from oscillatory, Friedel-like behavior. This potential has no empirical parameters and is valid at arbitrary temperature and density, yet it adds no additional computational complexity. We use this gradient-corrected screening potential to predict properties of warm dense matter that can be validated through XRTS experiments.

*liam@llnl.gov

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. LLNL-ABS-653177

Waves in a Lennard-Jones Dusty Plasma Liquid

M. Rosenberg[a] and G. J. Kalman[b]
[a]University of California, San Diego, La Jolla, CA 92093, U.S.A.
[b]Boston College, Chestnut Hill, MA 02467, U.S.A.

Generally, the interaction between negatively charged dust grains in three-dimensional (3D) dusty plasmas is modeled as a repulsive screened Coulomb (Yukawa) interaction, with the screening provided by the background lighter plasma particles. However, recently there have been methods proposed to "design" the binary interactions between charged dust particles by applying external ac electric fields to the dusty plasma [1-3]. The methods are based on the physical idea that the applied ac electric field would distort the Debye spheres of screening charges surrounding each dust grain, thereby changing the inter-grain interaction. This may lead to new binary interaction classes that could arise under uniaxial, biaxial or effective spherical polarization of the external ac electric fields [1-3]. It was shown theoretically that charged grains could interact via a Lennard-Jones type potential under the action of external ac fields with spherical polarization under certain conditions [3].

In this poster, we consider the dispersion of waves in the liquid phase of a 3D dusty plasma where the dust interacts via an isotropic Lennard-Jones potential. The theoretical approach uses the Quasi-Localized Charge approximation which requires input of the pair correlation function of the grains. Initially, we use an analytic expression for the pair correlation function of Lennard-Jones liquids from the literature. Preliminary results for the dispersion relations of both the longitudinal and transverse waves are presented. Possible dusty plasma parameters (probably under microgravity conditions) are discussed in which the rates of dissipative processes, such as dust-neutral or dust-dust collisions, are smaller than the characteristic dust wave frequencies.

Recognizing that the Lennard-Jones potential has been used as a model for interactions in liquid He [e.g., 4], we also discuss our results with reference to an experimental curve for (longitudinal) excitations in liquid He [5] that contain a "roton minimum." [6-7].

Work partially supported by NSF and NASA.

[1] A. V. Ivlev, G. E. Morfill, H. M. Thomas, et al., *Phys. Rev. Lett.* **100**, 095003 (2008).
[2] A. V. Ivlev, P. C. Brandt, G. E. Morfill, et al., *IEEE Trans. Plasma Sci.* **38**, 733 (2010).
[3] R. Kompaneets, G. E. Morfill and A. V. Ivlev, *Phys. Plasmas* **16**, 043705 (2009).
[4] P. A. Whitlock et al., *Phys. Rev. B* **19**, 5598 (1979).
[5] J. L. Yarnell et al., *Phys. Rev* **113**, 1379 (1959).
[6] K. I. Golden et al., *Phys. Rev. E* **82**, 036402 (2010).
[7] G. J. Kalman et al., *Europhys. Lett.* **90**, 55002 (2010).

Linear and quadratic static response functions of 3D Yukawa liquids

P. Magyar[1], Z. Donkó[1,2,*], G. J. Kalman[2], K. I. Golden[3]
[1]Wigner Research Centre for Physics, Budapest, Hungary
[2]Physics Department, Boston College, Chestnut Hill, USA
[3]Dept. of Mathematics and Statistics, Dept. of Physics, University of Vermont, Burlington, USA

The linear fluctuation-dissipation theorem (FDT) establishes a relationship between equilibrium two-point correlations in a system and its linear response to a small external perturbation. With increasing amplitude of the perturbation the response may become nonlinear: in this case the second or higher order response functions have to be considered. An extension of the conventional FDT to this regime is the *quadratic fluctuation-dissipation theorem* (QFDT) [1], which establishes a relationship between the quadratic response functions and the equilibrium three-point correlations. We study the linear and quadratic static density response functions of three-dimensional Yukawa liquids, $\hat{\chi}^{(1)}(\mathbf{k}_1)$ and $\hat{\chi}^{(2)}(\mathbf{k}_1, \mathbf{k}_2; \mathbf{k}_0)$, in molecular dynamics (MD) simulations, by applying a static external perturbation potential and measuring the induced density response. The response functions are generated from the equilibrium fluctuations via the FDT as well, by computing the static structure factors through separate, unperturbed equlibrium MD simulations. The figures show a very good agreement between the response functions, $\hat{\chi}^{(1)}(k_1)$ and $\hat{\chi}^{(2)}(k_1, k_1)$ on the one hand, and the associated static structure functions, $S(k_1)$ and $S(k_1, k_1)$, on the other.
Work partially supported by NSF and OTKA.

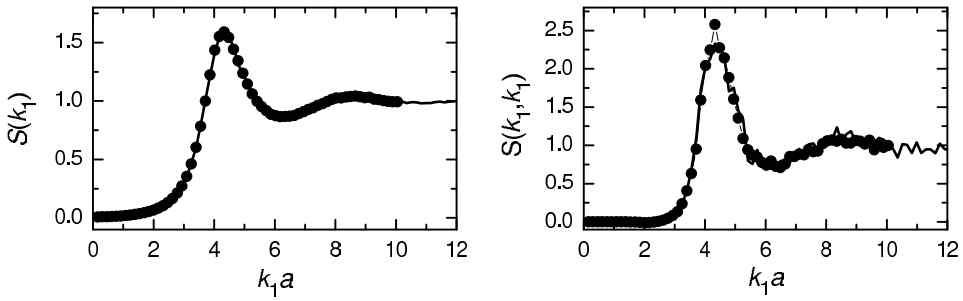


Figure 1: Linear $\hat{\chi}^{(1)}(k_1)$ and quadratic $\hat{\chi}^{(2)}(k_1, k_1)$ response functions for $\Gamma = 50$ and $\kappa = 1$ (symbols) and the corresponding structure functions $S(k_1)$ and $S(k_1, k_1)$ (thick lines).

*donko.zoltan@wigner.mta.hu

[1] K. I. Golden, G. J. Kalman, and M. B. Silevitch, J. Stat. Phys. 6, 87 (1972); A. G. Sitenko, Zh. Eksp. Teor. Fiz. 75, 104 (1978). [Sov. Phys. JETP 48, 5 (1978)].
[2] P. Magyar, Z. Donkó, G. J. Kalman, K. I. Golden, arXiv:1402.5797 [physics.plasm-ph]

Understanding the Difference between Transport in Strongly Coupled Quantum and Classical Plasmas

Paul E. Grabowski*
University of California, Irvine, Irvine, CA 92697, U.S.A.

Typical descriptions of transport in plasmas begin to break down as the Coulomb coupling parameter becomes large. Collisions begin to dominate, the screening length becomes of order the inter-particle spacing, potential energy can be as important as kinetic energy, and the electron density can become strongly localized around each ion. The importance of these effects can be understood via the quantum Boltzmann collision operator. I will characterize collisions as weak or strong and quantum or classical. The differences between a strongly coupled quantum and classical plasmas will be discussed and the errors in the classical and Born approximations will be quantified by comparing different approximations for the stopping power of ions. Resonances are particularly difficult for models to capture and play a different but strong roll in transport in both strongly coupled quantum and classical plasmas. Stopping power describes the energy loss of a projectile moving through a medium. This is just one of many transport properties that describe how energy flows through a plasma, but it is a velocity-resolved transport property; so stopping power is a strong test of kinetic theory models used to calculate transport. I will report how accurate different approximations are with respect to the full quantum Boltzmann equation derived stopping power.
*paul.grabowski@uci.edu

Optical emission diagnostics of plasma in a gaseous mixture of RF discharge

S.A. Orazbayev*, T.S. Ramazanov, M.K. Dosbolayev and M. Silamiya
Al Farabi Kazakh National University, IETP, al Farabi 71, Almaty, 050040, Kazakhstan.

Binary and multicomponent gaseous mixtures and substance vapors are used for solving many practical problems of physics. Varying of components of the gaseous mixture one can achieve results which cannot be obtained by using one component gases. Hense, the study of a separation phenomenon of the multicomponent gaseous mixture is interesting task of a nowadays, because it gives a knowledge about of redistribution degree dependence of the existence conditions of ionized gas.

Methods of optical diagnostics of plasma have a great development. These methods enable us to get extensive information about the plasma parameters and achieve a more detailed understanding of the physical processes in the system. Unlike the traditional methods of diagnosis the optical diagnostics is contactless and allows to determine different physical parameters of the plasma without affecting on it.

The experimental setup was described in detail in previous works [1-2]. The main elements of the experimental setup are two parallel electrodes between which the plasma is ignited. The upper one is grounded, the lower one is connected to the RF generator with frequency of 13.56 MHz. Diameters of both electrodes are 10 cm and distance between them is 3 cm. At the beginning of the experiment the working chamber is pumped out for a good vacuum to avoid discrepancies in studies. Argon, helium, hydrogen gases and their mixture were used as a working medium. The pressure of gases is varied in a region of 0.05-1.00 Torr and power of discharge in a region of 1 – 50 Watt.

The working chamber has lateral windows for monitoring processes in a plasma of RF discharge. The optical system for plasma diagnostics consists of the lens system and a spectrometer. The lens system is fixed so as to provide a clear image of interelectrode space on the entrance slit of the spectrometer.

The spectrum of Ar, He and H_2 gases were obtained by optical and spectral diagnostics method and also the electron temperatures were measured by obtained spectrum. Thus, the temperature of the electrons varies for Ar in range of 0.5 – 4 eV, for He in range of 2 – 7 eV, for H_2 in range of 1 – 5 eV, for Ar+He in range of 0.5 – 5 eV, at the pressure varying in the range of 0.1 – 1 Torr.

*sagi.orazbayev@gmail.com

[1] T. S. Ramazanov, A. N. Jumabekov, S. A. Orazbayev, M. K. Dosbolayev and M. N. Jumagulov // Phys. Plasmas. – 2012. №19. P. 023706.

[2] S. A. Orazbayev, M.M. Muratov, T. S. Ramazanov, M.K. Dosbolayev, M. Silamiya, M. N. Jumagulov, and L. Boufendi The Diagnostics of Dusty Plasma in RF Discharge by Two Different Methods // Contrib. Plasma Phys. – 2013. - V. 53, № 5. - P. 436 – 441.

Generalized Coulomb logarithm and energy loss of heavy particles in dense plasma

Kodanova S.K.*, Ramazanov T.S., Issanova M.K.
IETP, Al-Farabi Kazakh National University
71 Al-Farabi av., Almaty 050040, Kazakhstan

The precise knowledge of the energy loss of ions in ionized matter is important ащк both fundamental physics and applied research for inertial confinement fusion (ICF). The investigation of heavy high charged ions for inertial thermonuclear fusion requires qualitative and quantitative descriptions of the interaction of heavy particles with matter in a wide region of the densities and temperatures. One of the important values which describes the energy loss of the ions in plasma is the Coulomb logarithm. Many research areas, including ICF, dusty plasmas, plasma processing of materials, etc., use the formula $\lambda = Ln\Lambda$ for the Coulomb logarithm. However, this formula does not correctly account collisional processes and does not take into account the quantum effects in systems[1-3].

In this work the Coulomb logarithm is obtained by using effective potentials. These interaction potentials take into consideration lond-range many particle screening effects and short-range quantum-mechanical effects[4-5]. Using the method of spline approximation on the calculated data of the Coulomb logarithm, an interpolation formula for the Coulomb logarithm of electron-electron, electron-ion, ion-ion interactions is obtained. It should be noted that the interpolation formula correctly describes the theoretical results obtained by using effective potentials in a wide range of the coupling parameter Γ and the density parameter r_s. So, the expression obtained for the Coulomb logarithm interpolation formula could be used for calculations of dynamic properties of dense plasmas.

The Coulomb logarithms for protons (14.1 MeV), deuterons (12.5 MeV) and tritons (10.6 MeV) interacting with electrons and ions in DT plasma are calculated. It is shown, that the Coulomb logarithm on the basis of potentials which take into account diffraction effects is less than the level of the Coulomb logarithm $\lambda = \ln\Lambda$. We investigate the energy loss of heavy particles in DT plasma with a density higher than10^{20} cm^{-3}. Calculations of ions energy losses in the plasma for different values of the temperature and plasma density were carried out. Also, a comparison of the calculated data of ion stopping power with experimental and theoretical results of other authors was done.

*kodanova@physics.kz

[1] C.A. Ordonez, M.I. Molina. Evaluation of the Coulomb logarithm using cutoff and screened Coulomb interaction potentials.*Plasmas* 1, 2515 (1994)

[2] T.S. Ramazanov, S.K. Kodanova. Coulomb logarithm of a nonideal plasma.*Phys. Plasmas 8*, 5049 (2001)

[3] T.S. Ramazanov, S.K. Kodanova, Zh.A. Moldabekov.Dynamical properties of non-ideal plasma on the basis of effective potentials.*Phys. Plasmas 20*, 112702 (2013)

[4]T.S. Ramazanov, K.N.Dzhumagulova. Effective screened potentials of strongly coupled semiclassical plasma.*Phys. Plasmas 9*, 3758 (2002)

[5] T.S. Ramazanov, K.N. Dzhumagulova, and M.T. Gabdullin.Effective potentials for ion-ion and charge-atom interactions of densesemiclassical plasma.*Phys. Plasmas 14*, 042703 (2010)

2D One-Component and Binary Yukawa Systems in a Magnetic Field

T. Ott*[1], M. Bonitz[1], and H. Löwen[2]
[1]Institute for Theoretical Physics and Astrophysics
University of Kiel, Germany
[2]Institute for Theoretical Physics II: Soft Matter
University of Düsseldorf, Germany

A two-dimensional Yukawa system in a perpendicular magnetic field is considered. Computer simulations are carried out to explore the mobility (diffusivity) of one-component and charge-asymmetric binary systems. It is demonstrated that the mobility scales as the inverse of the magnetic field strength (Bohm diffusion) for strong fields. In binary systems, the ratio of the mobilities of the two species is tunable by the external magnetic field. It is furthermore shown that for large magnetic fields, the highly charged particles are practically immobile and form effective porous matrix for the other species.

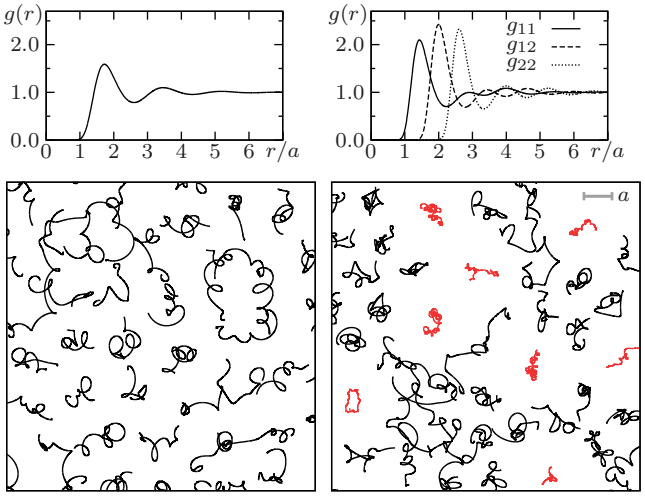


Figure 1: Pair distribution function and particle trajectories for $\omega_c/\omega_p = 0.5$ in a one-component system (left) and a binary system (right) at a charge ratio of 4. The more highly charged species is shown in red/gray.

*ott@theo-physik.uni-kiel.de

T. Ott, H. Löwen, and M. Bonitz. *Dynamics of two-dimensional one-component and binary Yukawa systems in a magnetic field.* Physical Review E, **89**, 0313105 (2014).

Gradient Corrections to the Exchange-Correlation Free Energy

Travis Sjostrom*
Los Alamos National Laboratory
Los Alamos, NM 87545, U.S.A.

In a recent work [1] a finite-temperature local density approximation (LDA) functional has been made available. In the present work we derive the first order gradient corrections to the exchange-correlation free energies of the homogeneous electron gas for use in finite temperature density functional theory (DFT) calculations. It is known that the gradient expansion at zero-temperature is often not better than LDA itself, however the only slightly more complex generalized gradient approximations (GGA, e.g. PBE [2]) have been successfully employed. We therefore consider finite temperature extension of the GGA functionals as well. These finite temperature functionals will be compared in self-consistent DFT calculations with each other and as well as with path integral Monte Carlo calculations, for which there is no approximation to the exchange-correlation.
*sjostrom@lanl.gov

[1] V.V. Karasiev, T. Sjostrom, J. Dufty, and S.B. Trickey, Accurate Homogeneous Electron Gas Exchange-Correlation Free Energy for Local Spin-Density Calculations, Phys. Rev. Lett. 112, 076403 (2014).
[2] J.P. Perdew, K. Burke, and M. Ernzerhof, Generalized Gradient Approximation Made Simple, Phys. Rev. Lett. 77, 3865 (1996).

Resolving Ultrafast Heating of Dense Cryogenic Hydrogen

U. Zastrau[1,2], P. Sperling[2,3]*, G. Gregori[4], S. Toleikis[5], T. Döppner[6], S. H. Glenzer[2], R. Redmer[3]

[1]Institut für Optik und Quantenelektronik, Friedrich-Schiller-Universität, D-07743 Jena, Germany

[2]SLAC National Accelerator Laboratory, Menlo Park CA 94025, USA

[3]Universität Rostock, D-18051 Rostock, Germany

[4]Department of Physics, Clarendon Laboratory, University of Oxford, Oxford OXI 3PU, United Kingdom

[5]Deutsches Elektronen-Synchrotron DESY, D-22607 Hamburg, Germany

[6]Lawrence Livermore National Laboratory, Livermore CA 94550, USA

Abstract

Free electron laser enable new pump-probe experiments to characterize warm dense matter, i.e. systems at solid-like densities and temperatures of several eV. Such extreme conditions are relevant for the interior of giant planets and along the compression path of inertial confinement fusion capsules. Of central importance for the generation and dynamics of warm dense matter are the electron-ion collision and equilibration time that determine the microscopic material properties. These times and consequently the dynamics of warm dense matter were studied within a pump-probe experiment [1] and will be presented here.

We will report on the dynamics of ultrafast heating in cryogenic hydrogen initiated by a $\lesssim 300$ fs, 92 eV free electron laser x-ray burst. The rise of the x-ray scattering amplitude from a second x-ray pulse probes the transition from dense cryogenic molecular hydrogen to a nearly uncorrelated plasma-like structure, indicating an electron-ion equilibration time of ~ 0.9 ps. The rise time agrees with radiation hydrodynamics simulations based on a conductivity model for partially ionized plasma that is validated by two-temperature density-functional theory.

*philipp.sperling@uni-rostock.de

[1] U. Zastrau *et al.*, *Resolving Ultrafast Heating of Dense Cryogenic Hydrogen*, Phys. Rev. Lett. **112**, 105002 (2014).

Thermodynamics of shock and isentropically compressed hydrogen and helium at megabar pressure range

V.E. Fortov[1,2]*, V.K. Gryaznov[1] and I.L. Iosilevskiy[2,3],

[1]Institute of Problems of Chemical Physics RAS, 141432, Chernogolovka, Russia
[2]Joint Institute for High Temperatures RAS, 125412 , Moscow, Russia
[3]Moscow Institute of Physics and Technology (State University), 141700, Moscow, Russia

Comparison of theoretical predictions and recently obtained experimental data on shock and isentropic compression of hydrogen and helium in megabar and multi-megabar pressure range is under discussion. Firstly it is high-explosive (HE) adiabatic (quasi-isentropic) compression of deuterium and helium up to ~ 50 Mbar (Mochalov et al.[1]) and shock compression of pre-compressed gaseous deuterium up to ~2 Mbar and 1.1 g/cc (Leubeyre et al.[2]). We use for comparison the same thermodynamic model (SAHA-code, Gryaznov et al.[3]), which was successful previously for description of shock and adiabatic compression of solid and porous metals, condensed and pre-compressed gaseous deuterium (hydrogen), helium and rare gases in megabar pressure range. Thermodynamics for all these materials was described via SAHA-model as an equilibrium multi-component strongly coupled mixture of atoms, molecules, ions and electrons ("chemical picture") with taking into account of modified Coulomb corrections, corrections for intensive short-range repulsion of heavy particles, and strong degeneracy effects of free electrons. Satisfactory agreement between new experimental data and theoretical prediction was achieved both in pressure-density and temperature-density planes. Equilibrium ionization and dissociation composition along adiabats of compression, as well as influence of Coulomb nonideality and electronic degeneracy effects are revealed and discussed in conditions of the greatest pressure presently obtained in scientific laboratory.

*fortov@ihed.ras.ru

[1] M.A. Mochalov, R.I. Il'kaev, V.E. Fortov et al. // Experimental study of quasi-isentropic compression of deuterium and helium at pressure 1500…5000 GPa. *JETP*, 2014 (to be published).

[2] P. Loubeyre, S. Brygoo, J. Eggert et al. // Extended data set for the equation of state of warm dense hydrogen. *Phys. Rev.* B, **86**, 144115 (2012).

[3] Gryaznov, V., Iosilevskiy, I., Fortov V. // Equation of state of shock compressed gases at megabar pressure range. *Proceedings of APS-2011*, AIP, Conf. Ser. **1426,** 917 (2012).

Superdiffusion of 2D Yukawa Liquids Due to a Perpendicular Magnetic Field

Yan Feng[1]*, J. Goree[2], B. Liu[2], T. Intrator[1], and M. S. Murillo[1]
1. Los Alamos National Laboratory, Los Alamos, NM 87545, U.S.A.
2. Dept. of Physics & Astronomy, The Univ. of Iowa, Iowa City, IA 52242, U.S.A.

Normal and anomalous diffusion of 2D strongly coupled dusty plasmas without magnetic fields have been studied both theoretically and experimentally in the past decade. The particle motion can be characterized using mean-squared displacement (MSD), defined as $\langle|\mathbf{r}_i(t) - \mathbf{r}_i(0)|^2\rangle$. In the log-log plot, if the MSD curve fits a straight line with a slope α, then the MSD obeys a power law $\propto t^{\alpha}$. Normal diffusion is characterized by $\alpha = 1$, while superdiffusion and subdiffusion are characterized by $\alpha > 1$ and $\alpha < 1$, respectively. Recently, dusty plasma behaviors under magnetic fields have attracted attention, especially the Magnetized Dusty Plasma (MDPX) facility. A very strong magnetic field is needed to magnetize strongly coupled dusty plasma, with comparable cyclotron and plasma frequencies for dust particles. The gyro motion of dust particles due to the applied magnetic field may drastically change the collective dynamics of dusty plasmas. Here, Langevin dynamics simulations of thousands of particles, including both driven and dissipation from the surrounding plasma gas, were performed to study the diffusion of individual charged particles of 2D Yukawa liquids, with a magnetic field perpendicular to the 2D plane. The gyro motion is competing with the thermal motion, and as a result, the diffusion behavior of individual particles will be suppressed by the applied magnetic field. As diagnostics of diffusion, the MSD (shown in Fig.1) and velocity autocorrelation function have been calculated from the simulated particle trajectories. Our simulation results suggest that, when the external magnetic field is high enough so that β (the ratio of the cyclotron and plasma frequencies for dust particles) is close to 1, the motion of dust particles tends to be more superdiffusive, as the exponent α reaches 1.1 (shown in Fig.2).

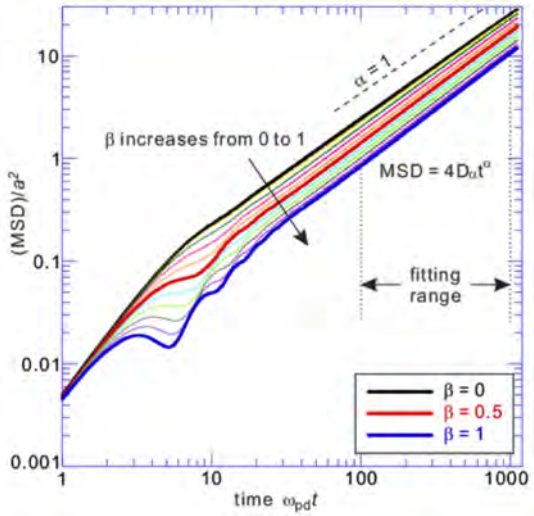


FIG. 1: Mean-squared displacement (MSD) as a function of time, averaged over many particles. In this log-log plot, the slope corresponds to the exponent α in a power law.

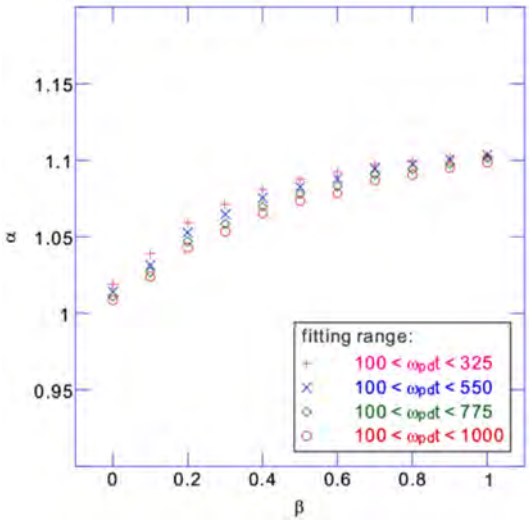


FIG. 2: The fitting results of exponent α, shown as a function of the dimensionless magnetic field β.

Work supported by DOE, NSF and NASA.
*yfeng@lanl.gov

Enhancement of stopping power in dense two-component plasmas

Yu.V. Arkhipov, A.B. Ashikbayeva, A. Askaruly, A.E. Davletov, D. Dubovtsev
Department of Physics and Technics, IETP, al-Farabi Kazakh National University
Al-Farabi av. 71, Almaty 050040, Kazakhstan
I.M. Tkachenko*
Instituto de Matemática Pura y Aplicada, Universidad Politécnica de Valencia
Camino de Vera s/n, 46022 Valencia, Spain

It is well known[1] that the plasma polarizational stopping power is traditionally calculated by integrating the inverse dielectric function $\epsilon^{-1}(k,\omega)$ of a simple electron fluid. For a two-component plasma the influence of the target ions on the Bethe-Larkin asymptotic form of the stopping power manifests itself in the Langmuir plasma mode long-wavelength upshift which is closely related to the fourth power frequency moment of the plasma loss function[2], $\left(-\operatorname{Im}\epsilon^{-1}(k,\omega)/\omega\right)$. Note that the power frequency moments of the plasma loss function are expressed in terms of the partial static structure factors which can be calculated using various theoretical approaches such as the Ornstein-Zernike relation in the hyper-netted chain approximation. In the present work the Nevanlinna theorem of the theory of moments[3] is applied to reconstruct the loss function of a two-component dense plasma and, then, the polarizational stopping power is evaluated to demonstrate that the interaction between the target electron and ion components enhances the stopping of heavy projectiles penetrating the plasma medium. It is shown herein that a similar result holds for some other known models of the two-component plasma dielectric function, like the extended Born-Mermin model[4] generalized to non-zero temperatures.

*imtk@mat.upv.es

[1] J. Lindhard. *On the properties of a gas of charged particles.* K. Dan Vidensk. Selsk. Mat. Fys. Medd., **28(8)** 1, (1954).

[2] D. Ballester, I.M. Tkachenko. *Fast-Projectile Stopping Power of Quantal Multicomponent Strongly Coupled Plasmas.* Phys. Rev. Lett., **101** 075002, (2008).

[3] I.M. Tkachenko, Yu.V. Arkhipov, A. Askaruly. *The Method of Moments and its Applications in Plasma Physics.* LAMBERT Academic Publishing, Saarbrucken, Germany, (2012).

[4] C. Fortmann, A. Wierling, and G. Ropke. *Influence of local-field corrections on Thomson scattering in collision-dominated two-component plasmas.* Phys. Rev. E, **81** 026405, (2010).

SCCS 2014
Abstracts

Wednesday, July 30th

A review of studies on Strongly-Coupled Coulomb Systems since the rise of DFT and the inaugural SCCS-meeting in 1977.

M. W. C. Dharma-wardana, National Research Council of Canada
Ottawa, Canada, K1A 0R6.

The conferences on "strongly coupled Coulomb systems" (SCCS) began as the seminal "Strongly coupled Plasmas" conferences, with the inaugural volume edited by Kalman and Carini. This year (2014) is also the centenary of the Ornstein-Zernike equation of classical statistical mechanics. Here we review the progress in SCCS, mostly within our own involvement in the subject, jointly with François Perrot. We attempted to use density functional theory (DFT) as well as classical integral equations (viewed as a part of DFT) in a self-consistent manner for SCCS at finite-T. Green's function methods were used to support such investigations. Initially, the interest was in extending the theory of weakly-interacting classical Coulomb systems to strongly interacting systems for which Molecular-Dynamics began to be available. Meanwhile, Thomas-Fermi models and simple ion-sphere models had reached their limit of usefulness for quantum SCCS. DFT was poised to dominate condensed mater physics, mainly at $T = 0$. General Coulomb systems contain a mixture of electrons and ions at finite-T, where the ions are practically classical, while the electrons are quantum mechanical (forming bound-states) near nuclei, while showing near-classical behaviour far from nuclear centers. The ion-sphere models of Salpeter, Rosznyai and others treated such matters, and evolved into useful average-atom models as in David Lieberman's *Inferno* models and more recent *Purgatorio* models. Ion-sphere models were replaced by *correlation-sphere models* by Dharma-wardana and Perrot to take advantage of the description of matter *via* pair-distribution functions. While the SCCS series covers many topics including astrophysics, dusty plasmas etc., we limit this review to some topics that we have worked on, viz., (a) construction of pseudopotentials and exchange-correlation functionals for finite-T Coulomb systems; (b) equation of state over many orders of temperature and density; (b) spectroscopy, opacity (line widths, microfields, ionization and brehmstrahlung), scattering; level shifts and continuum edges; (c) transport properties, e.g., static and dynamic conductivity; (d) laser- and shock- created plasmas, their temperature relaxation and transient (optical and transport) properties; (e) Search for simpler computational schemes, essentially classical maps, for dealing with SCCS. The latter has proceed *via* searches for orbital-free DFT, and *via* classical integral equations (e.g., Ornstein-Zernike, Hyper-netted-Chain) and pair-potentials constructed to capture quantum effects. Laughlin's plasma map for the fractional quantum Hall effect is a celebrated example of the latter. Here we present its extension to graphene. Progress in these topics in the context of finite-T SCCS will be reviewed.
*chandre.dharma-wardana@nrc-cnrc.gc.ca

Wednesday Talks

Plasmons and Screening in Electron Systems with Internal Degrees of Freedom

John Schliemann

Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany

I will report on recent studies of the dielectric function evaluated within random phase approximation for electron liquids with nontrivial (pseudo-)spin degrees of freedom. The systems considered include heavy and light holes in III-V semiconductors [1,2], graphene [3], and molybdenum disulfide [4].

*John.Schliemann@physik.uni-regensburg.de

[1] J. Schliemann, Phys. Rev. B **74**, 045214 (2006); Europhys. Lett. **91**, 67004 (2010); Phys. Rev. B **84**, 155201 (2011).
[2] A. Scholz, T. Dollinger, P. Wenk, K. Richter, and J. Schliemann, Phys. Rev. B **87**, 085321 (2013).
[3] T. Stauber, J. Schliemann, and N. M. R. Peres, Phys. Rev. B **81**, 085409 (2010); A. Scholz and J. Schliemann, Phys. Rev. B **83**, 235409 (2011); A. Scholz, T. Stauber, and J. Schliemann, Phys. Rev. B **86**, 195424 (2012).
[4] A. Scholz, T. Stauber, and J. Schliemann, Phys. Rev. B **88**, 045118 (2013).

Relaxation dynamics of strongly correlated fermions in lattice systems

M. Bonitz[1], S. Hermanns[1], C. Hinz[1], , N. Schlünzeb[1] and D. Lacroix[2]
[1]Institute for Theoretical Physics and Astrophysics,
Christian Albrechts University Kiel,
24098 Kiel, Germany
[2] IPN Orsay, 15 Rue Georges Clemenceau, 91406 Orsay

With the growing availability of intense short-pulse radiation sources it becomes possible to drive interacting many-particle or few-particle systems out of equilibrium in a controlled way. The subsequent relaxation and equilibration dynamics is still poorly understood, in particular, for fermions. From a theory point of view these processes are complicated due to the simultaneous dynamics of the occupation functions and of binary correlations. The problem becomes even more complicated when the system has finite size and is spatially inhomogeneous [1].
The Hubbard model is a prototype for treating correlation effects in condensed matter or optical lattices fully including finite size and inhomogeneity effects. We, therefore, concentrate on the relaxation dynamics of small 1D, 2D and 3D Hubbard clusters that contain from a few to several hundred electrons. We observe a complex multi-stage relaxation behavior that depends on the external excitation, on the coupling strength and on the geometry of the system.
We present results from two complementary theoretical approaches: first, from nonequilibrium Green functions where we apply the Generalized Kadanoff Baym ansatz [1, 2] and, second, from a stochastic mean field approach [3] that was recently developed in nuclear physics [4].
*bonitz@physik.uni-kiel.de

[1] K. Balzer, and M. Bonitz, *Nonequilibrium Green's Functions Approach to Inhomogeneous Systems*, Lecture Notes in Physics, vol. 867 (2013)
[2] S. Hermanns, and M. Bonitz, subm. to PRB (2014), arXiv:1402.7300
[3] D. Lacroix, S. Hermanns, C. Hinz, and M. Bonitz, subm. to PRL (2014), arXiv:1403.5098
[4] S. Ayik, Phys. Lett. B 658, 174 (2008)

Structure of Two-Dimensional Plasma Crystals in Anharmonic Penning Traps.

Daniel H. E. Dubin
Dept. of Physics
UC San Diego La Jolla CA 92093

In several recent experiments charged particles have been trapped and cooled in two-dimensional (2D) crystalline configurations using a Penning trap. Usually in such traps the applied trap potential is harmonic (i.e. depending quadratically on position), and consequently the 2D crystal structure is nonuniform and riddled with defects throughout. This poster derives a closed-form analytic expression for the density per unit area of the 2D crystal when an arbitrary anharmonic trap potential is employed, expressed as a multipole expansion. This expression is used to find the optimum potential, with a given number of multipoles, for trapping a plasma crystal with the most uniform possible density per unit area. Image charge effects are included to lowest order in (plasma size)/(electrode radius). Minimum energy crystalline states in such an optimized trap potential (including only quadrupole and octopole terms) are evaluated numerically and the resulting crystals are shown to be defect-free over the central region where the density is most nearly uniform. The poster also explores using an $l = 3$ rotating wall trap potential in order to produce near-perfect crystals with triangular boundaries and no defects whatsoever.[1]

Supported by PHY-0903877 and DE-SC0002541.

[1]D.H.E. Dubin, Phys Rev A 88, 013403 (2013).

Quantum Effects and Shell Structure for Confined Charges

James Dufty* and Jeff Wrighton
Department of Physics
University of Florida, Gainesville, FL 32611

Sandipan Dutta
Asia Pacific Center for Theoretical Physics
Pohang, Kyongsang-bukto, Korea

A recently developed method for mapping an equilibrium quantum system to an equivalent classical system [1] is applied to the calculation of density profiles for harmonically confined charges over a wide range of temperatures. Quantum effects in the classical representation appear via a modification of the intensity of the Coulomb pair interaction and a change in the shape of the confining potential. Different origins of shell structure at high and low temperatures are demonstrated. In the classical limit of high temperatures and low densities shell formation requires strong Coulomb correlations. In the opposite limit of low temperatures and high density the effective Coulomb coupling is weaker and shell structure is dominated by strong exchange correlations (quantum statistics). More generally, there is a continuous cross-over between these two mechanisms. The classical many-body analysis is implemented via liquid state theory (hypernetted chain approximation) and classical Monte Carlo simulation.

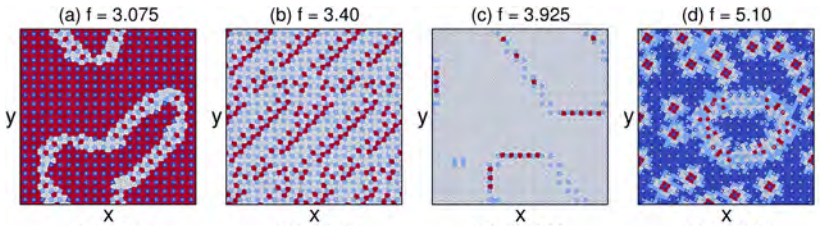
*duftyjim@gmail.com

[1] J. W. Dufty and S. Dutta, Contrib. Plasma Phys. 52 100 (2012); Phys. Rev. E 87 032101 (2013); S. Dutta and J. Dufty, Phys. Rev. E 87, 032102 (2013); Euro. Phys. Lett., 102 67005 (2013).

Interacting Coulomb Systems on Periodic and Quasiperiodic Substrates: Applications in Dusty Plasmas, Soft Matter Systems, and Materials Science

C. Reichhardt* and C.J.O. Reichhardt
Los Alamos National Laboratory
Los Alamos, CA 87544, U.S.A.

There are many examples of collectively interacting particles systems that form a crystalline structure through mutually repulsive interactions, such as Coulomb or Wigner crystals, dusty plasmas, charge-stabilized colloidal assemblies, vortices in type-II superconductors, and charge density wave systems. Here we examine how such systems behave in the presence of crystalline or quasicrystalline substrates, which can induce a rich variety of static and dynamic behaviors due to the competition between the triangular ordering favored by the particle-particle interactions and the ordering imposed by the substrate. These include commensurate and incommensurate phases, which occur when the length scale of the particle lattice matches or dos not match an integer or rational fraction of the substrate length scale. For incommensurate phases we find a rich variety of novel structures such as stripes, checkerboards, domain walls, and glassy phases. We also observe a series of transitions from triangular lattice to square lattice and superlattice states[1]. Under an applied drive we find a remarkable variety of dynamical phenomena such as the flow of soliton-like excitations, dynamic pattern formation, and nonequilibrium phase transitions between different flowing states[2]. The nature of the dynamical response varies depending on whether the system is commensurate or incommensurate. We also examine the effect of driving the particles over quasicrystalline substrates and find disordered states for some drive angles with locking into moving ordered lattice states for driving along and close to effective symmetry directions of the substrate[3]. We compare our results to recent experiments performed for particles with Yukawa interactions on periodic substrates[4,5].



*reichhardt@lanl.gov

[1] D. McDermott, J. Amelang, L.M. Lopatina, C.J. Olson Reichhardt, and C. Reichhardt, Domain and Stripe Formation Between Hexagonal and Square Ordered Fillings of Colloids on Periodic Pinning Substrates. *Soft Matter*, 9:4607, 2013.

[2] D. McDermott, J. Amelang, C.J. Olson Reichhardt, and C. Reichhardt, Dynamic Regimes for Driven Colloidal Particles on a Periodic Substrate at Commensurate and Incommensurate Fillings. *Physical Review E,* 88:062301, 2013.

[3] C. Reichhardt and C.J. Olson Reichhardt, Dynamical Ordering and Directional Locking for Particles Moving Over Quasicrystalline Substrates. *Physical Review Letters,* 106:060603, 2011.

[4] T. Bohlein, J. Mikhael, and C. Bechinger, Observation of Kinks and Antikinks in Colloidal Monolayers Drive Across Ordered Surfaces. *Nature Materials*, 11:126, 2012.

[5] T. Bohlein and C. Bechinger, Experimental Observation of Directional Locking and Dynamical Ordering of Colloidal Monolayers Driven Across Quasiperiodic Substrates. *Physical Review Letters* 109:058301, 2012.

Excitonic condensation in double-bilayer graphene

S. De Palo[2,1] and G. Senatore*[1,2]

[1]Dipartimento di Fisica, Università di Trieste, strada Costiera 11, 34151 Trieste, Italy

[2]CNR-IOM-Democritos, Trieste, Italy.

We investigate the excitonic condensation in symmetric double-bilayer graphene, at densities for which the independent electron dispersion in each bilayer is quadratic and with the two bilayers respectively doped with electrons and holes. We build on the study of [1,2], in which a mean field approach with effective RPA like inter-particle interactions is used and only inter-layer interactions are included, either with normal state or symmetry-broken state screening. We extend the previous investigation by employing the full RPA response matrix of the bilayer to construct the inter- and intra-layer effective interactions that we use in the mean field approach. The limit in which the valley degeneracy of the bilayers is neglected allows for a check of the accuracy of the combined approximations, thanks to the mapping onto the symmetric electron-hole bilayer, for which QMC simulations are available [3,4]. If time permits, we shall also illustrate the predictions of an alternative, self-consistent approach. This is based on the RPA energy functional built from the broken-symmetry state of a non-interacting system in a symmetry-breaking field; the amplitude of such field provides the selfconsistent parameters. This approach, which is inspired by [5], constitutes a Landau-Fermi liquid scheme for symmetry broken states.

*senatore@units.it

[1] A. Perali, D. Neilson, and A. R. Hamilton, Phys. Rev. Lett. **110**, 146803 (2013).

[2] D. Neilson,1 A. Perali, and A. R. Hamilton Phys. Rev. BR**89**,060502 (2014).

[3] S. De Palo, F. Rapisarda, and G. Senatore, Phys. Rev. Lett. **88**, 206401 (2002).

[4] R. Maezono, P. Lopez Rios, T. Ogawa, and R. J. Needs, Phys. Rev. Lett. **110**, 216407 (2013).

[5] P. Nozieres and C. Comte, J. Physique **43** 1083 (1982).

Thermodynamic properties of the homogeneous electron gas - a Configuration Path Integral Monte-Carlo approach

T. Schoof*, S. Groth, A. Filinov, and M. Bonitz
Institute for Theoretical Physics and Astrophysics,
Christian Albrechts University Kiel, Germany

Thermodynamic properties of the homogeneous electron gas (HEG) at finite temperatures are of high importance for many systems, including warm dense matter or astrophysical plasmas. Recently, Restricted Path Integral Monte-Carlo (RPIMC) data for low to moderate densities have been presented [1], while the high density regime was not accessible due to the Fermion sign problem. However, accurate data over a full range of densities are of great interest, e.g., for numerical modeling serving as input to DFT calculations [2].
Here we apply the recently developed Configuration PIMC (CPIMC) method to the HEG at high densities ($r_s < 1$) and low to moderate temperatures ($\Theta \leq 1$). The CPIMC method allows for the efficient ab-initio calculation of thermodynamic properties of highly degenerate, moderately coupled systems [3,4]. It is based on the representation of the N-particle density operator in a basis of antisymmetrized N-particle states (configurations of occupation numbers) and does not suffer from the Fermion sign problem in the non-interacting limit.

*schoof@theo-physik.uni-kiel.de

[1] E. W. Brown, B. K. Clark, J. L. DuBois, and D. M. Ceperley, Phys. Rev. Lett. **110**, 146405 (2013).

[2] V. V. Karasiev, T. Sjostrom, J. Dufty, and S. B. Trickey, Phys. Rev. Lett. **112**, 076403 (2014).

[3] T. Schoof, M. Bonitz, A. Filinov, D. Hochstuhl, and J. Dufty, Contrib. Plasma Phys. **51**, 687 (2011).

[4] T. Schoof, S. Groth and M. Bonitz in *Complex Plasmas: Scientific Challenges and Technological Opportunities*, edited by M. Bonitz, K. Becker, J. Lopez and H. Thomsen, Springer, in press (2014)

Strongly Coupled Ultracold Plasmas from Rydberg Blockaded Gas of Ultracold Atoms

Gautham Dharuman,[1] Michael S. Murillo,[2,*] John Verboncoeur[1] and Andrew Christlieb[1]

[1]Michigan State University, East Lansing, MI 48824, U.S.A.

[2]Los Alamos National Laboratory, Los Alamos, NM 87545, U.S.A.

Ultracold plasmas were originally created by photoionizing a gas of ultracold atoms. Because of the low electron and ion temperatures (micro- to milli- Kelvin), the (neutral) plasma can be strongly coupled. Despite the enormous initial coupling, it was shown that the coupling parameter rapidly decreases to near unity due to the process of Disorder-Induced-Heating (DIH)[1] that is inevitable in a plasma formed by ionizing a disordered gas of ultracold atoms. However, one of the applications of the ultracold plasma is in high-brightness ion beam technology[2] for nanofabrication and characterization which requires plasmas with stronger coupling. This requires mitigation of DIH and it was predicted that this is possible if the initial ion system, just after ionization, is correlated[3]. There are a number of ways of preparing an initially correlated state, of particular interest is the Rydberg blockaded gas of ultracold atoms where the Rydberg blockade effect results in correlations between the Rydberg atoms. A recent experiment[4], demonstrated the delay in ionization of the Rydberg gas as a result of the blockade effect thereby suggesting the possibility that the plasma formed could be strongly coupled. This work focusses on the study of the effects of strong correlation in the creation and evolution of the plasma through molecular dynamics simulation with explicit ions and explicit electrons. To explicitly treat electron dynamics, without complete quantum mechanical treatment, effective quantum potentials in the form of momentum-dependent pseudo-potentials[5] are used in classical simulations. These potentials incorporate the effects of the Heisenberg Uncertainty Principle and the Pauli Exclusion Principle through classical phase space exclusion. The extent of exclusion is determined by a set of parameters that are found to be elliptically correlated for ground state atomic energies that match Hartree-Fock values. From our molecular dynamics simulations we attempt to optimize the final coupling value.

*murillo@lanl.gov

[1] M. Lyon, S. D. Bergeson and M. S. Murillo, Limit of strong ion coupling due to electron shielding, *Phys. Rev. E* **87**, 033101 (2013).

[2] J. L. Hanssen, S. B. Hill, J. Orloff and J. J. McClelland, Magneto-Optical-Trap-Based High Brightness Ion Source for Use as a Nanoscale Probe, *Nano Lett.* **8**, 2844 (2008).

[3] M. S. Murillo, Using Fermi Statistics to Create Strongly Coupled Ion Plasmas in Atom Traps, *Phys. Rev. Lett.* **87**, 115003 (2001).

[4] M. R. Vincent, C. S. Hofmann, H. Schempp, G. Gunter, S. Whitlock, and M. Weidemuller, Spontaneous Avalanche Ionization of a Strongly Blockaded Rydberg Gas, *Phys. Rev. Lett.* **110**, 045004 (2013).

[5] J. S. Cohen and L. Wilets. Fermion Molecular Dynamics in Atomic, Molecular and Optical Physics. *Contemp. Phys*. **39,** 163 (1998).

Work supported by the Air Force Office of Scientific Research (AFOSR).

Rydberg Matter and Ultracold Plasma.

B.B. Zelener[1, 2]*,A. A. Bobrov[1], M.A. Butlitsky[1], S. Y. Bronin[1], D. R. Khikhlukha[1], V.A. Sautenkov[1,4],S. A. Sahakian[1], E.A. Manykin[2, 3], B.V. Zelener[1],V.E. Fortov[1]

[1] Joint Institute for High Temperatures of Russian Academy of Sciences, Moscow, 125412, Russia

[2] National Research Nuclear University, Moscow, 115409, Russia

[3] Kurchatov Institute, National Research Centre, Moscow, 123182, Russia

[4] P. N. Lebedev Physical Institute of Russian Academy of Sciences, Moscow, 119991, Russia

In my presentation I will discuss our theoretical analysis of thermodynamical and kinetics properties of ultracold rydberg atoms and plasma[1,2]. In our simulations we use Monte-Carlo and molecular dynamics techniques. Reduction of plasma recombination and creation of regular structure are demonstrated under strong interaction condition. Magnetic field can help dramatically reduce the recombination plasma rate. We have assembled an experimental setup for preparation and study of ultracold lithium plasma[3]. Also I will present recent experimental results.

This work was supported by grants from the Program for basic research of the Presidium of the Russian Academy of Sciences Study of matter under extreme conditions under the guidance of Academic Fortov V.E., President Grant of Russian Federation MK-4092.2014.2, Russian Fundation of Basic Research Grant 14-02-00828.

*bobozel@mail.ru

[1] A. A. Bobrov, S. J. Bronin, B. B. Zelener, B. V. Zelener, E. A. Manykin, D. R. Khikhlukha, “Electron distribution function and recombination coefficient in ultracold plasma in a magnetic field”, *JOURNAL OF EXPERIMENTAL AND THEORETICAL PHYSICS*, 117, 1, 161 (2013)

[2] E. A. Manykin, B. B. Zelener, B. V. Zelener, “Thermodynamic and kinetic properties of nonideal Rydberg matter”, *JETP LETTERS*, 92, 9, 630 (2011)

[3] B. B. Zelener, S. A. Saakyan, V. A.Sautenkov, *et al.* “Laser cooling of Li-7 atoms in a magneto-optical trap”, *JETP LETTERS*, 98, 11, 670 (2014)

Fano-like resonances in strongly coupled Coulomb systems

L. Silvestri[1], G. J. Kalman[1], Z. Donko[1,2], P. Hartmann[1,2], H. Kaehlert[1,3]
[1]Boston College, Chestnut Hill, MA 02467, USA
[2]Wigner Research Centre for Physics, Budapest, Hungary
[3]Institut fur Theoretische Physik and Astrophysik, Kiel, Germany

Molecular Dynamics (MD) simulation of a strongly coupled binary ionic mixture has revealed the presence of a sharp minimum of several orders of magnitude in the dynamical density (current) fluctuation spectrum of the system. This phenomenon is reminiscent of the well-known Fano anti-resonance observed in various physical systems, first analyzed in the pioneering work of Ugo Fano on spectral profiles. Recently, it has been pointed out that the Fano resonance effect can be understood on the basis of a classical model as a feature of the response function of a multi-resonant system, and therefore it is a phenomenon that should occur in classical systems as well. What, however, is not widely recognized is that there must be a corollary to this phenomenon as demanded by the Fluctuation Dissipation Theorem: the equilibrium fluctuation spectrum of a strongly coupled system has to display a similar spectral feature. We present a theoretical description based on the Quasi Localized Charge Approximation, reformulated to include collisional effects, in order to explain the simulation results. The essence of the phenomenon is that the minimum is due to the interference between the two damped plasmon modes of a binary system. The validity of the theoretical model has been verified by further MD simulations and an excellent agreement between theory and observation has been demonstrated, showing the existence of this novel manifestation of the Fano theory.

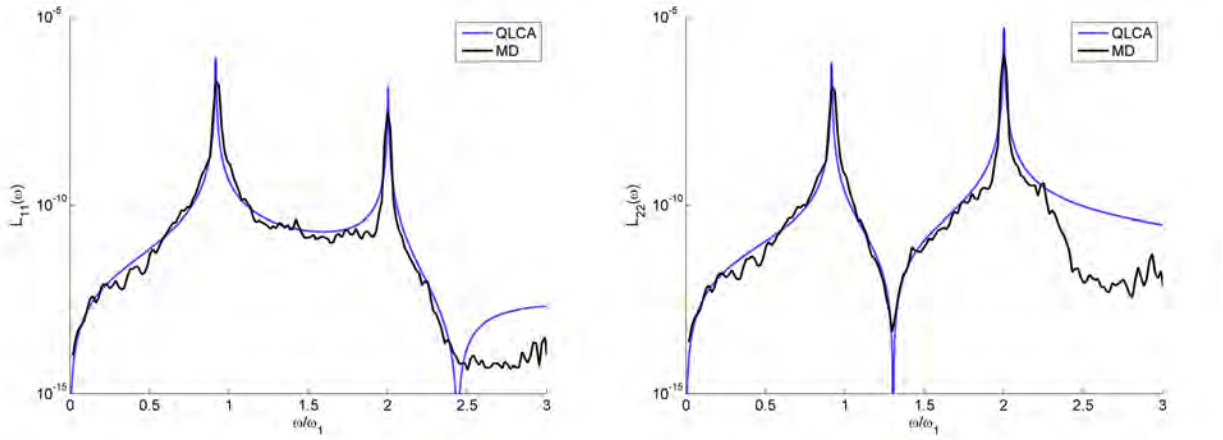


Figure 1. Comparison between MD simulation (solid black line) and the extended QLCA model (dashed blue line) of the dynamical current-current correlation spectra in the crystalline phase for each of the two species, (left) L_{11}, (right) L_{22}. The system was characterized by the charge $Z = Z_2/Z_1 = 0.7$ mass $m = m_2/m_1 = 0.2$, density $\rho = n_2/n_1 = 1$ ratios.

*silveslu@bc.edu

Wednesday Talks

SCCS 2014
Abstracts

Thursday, July 31st

Fundamental Science Experiments on the National Ignition Facility*

T. Doeppner
Lawrence Livermore National Laboratory
Livermore, CA 94551, U.S.A.

The National Ignition Facility (NIF) has been in operation for five years. First experiments during the National Ignition Campaign (NIC) were focused on achieving ignition in the laboratory. For this purpose, 192 laser beams deliver up to 1.9 MJ energy at up to 500 TW peak power in precisely-tuned pulse shapes into a gold hohlraum, a cylindrically shaped radiation cavity, that converts the laser energy into a nearly Planckian X-ray bath to indirectly drive and implode the fuel capsule at the center of the hohlraum. Early experiments were geared towards bringing up diagnostic capabilities at the NIF and developing a wide range of tuning platforms. Thanks to these early achievements, in recent years the applications on the NIF have multiplied and, among others, a growing fundamental science program has been established that enables facility access to outside users.

In my talk I will first briefly review progress on the path towards ignition. In recent fully integrated implosion experiments it was demonstrated that by increasing the first-shock strength, which comes at the cost of setting the fuel at a higher adiabat, the implosions become less susceptible to hydrodynamic instabilities. This resulted in significantly improved performance with fusion yield for the first time exceeding the energy absorbed by the deuterium-tritium fuel [1] and a significant portion of the yield being the result from additional hot spot heating thanks to alpha particle stopping.

In the second part of my talk I will present the results of a series of fundamental science experiments at the NIF aiming at absolute equation of state (EOS) and opacity measurements of CH plastic along the principal Hugoniot at unprecedented pressures approaching 1 Gbar [2]. Such experiments are important to benchmark atomic physics models and improve simulations of indirectly-driven ICF implosions in which CH currently is the primary ablator material. In these experiments, a hohlraum drive with 290 eV peak radiation temperature, launches a strong shock wave into a 2.2 mm diameter plastic ball. The induced pressures by the spherical shock wave increase as the shock converges allowing to obtaining a range of Hugoniot states in a single experiment. Pressures reach ~ 1 Gbar as the shock wave coalesces at the center of the CH target. We measure the radiography contrast at the shock front with a powerful Zn He-alpha backlighter source to infer compression. The opacity along the Hugoniot is also deduced, which is essential in Gbar experiments as it changes significantly from its initial value due K-shell ionization of carbon. The first experiments achieved pressures up to 720 Mbar, which is an order of magnitude greater than previously measured in CH [3]. The measured EOS locus was consistent with the previous measurements, and significantly stiffer than the theoretical EOS used for comparison. Our analysis also gave the variation of opacity along the Hugoniot, which showed a decrease of an order of magnitude, approximately as expected from atomic physics calculations.

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

**email: doeppner1@llnl.gov

[1] O. Hurricane et al., Nature **506**, 343–348 (2014).
[2] A. Kritcher et al., High Energy Density Physics **10**, 27 (2014).
[3] R. Cauble et al., Phys. Rev. Lett. 80, 1249 (1998).

Laboratory Studies of Warm Dense Matter with High Power Lasers and 4th Generation Light Sources

G. Gregori*
Department of Physics, University of Oxford
Oxford, OX1 3PU, United Kingdom

The combination of high power optical lasers and free electron lasers operating at short wavelength (in the x-ray regime) has opened new avenues for laboratory astrophysics, where exotic states of matter can now be generated and probed with high accuracy. We will review a few examples of recent experiments performed at high power laser facilities (the Titan laser at Lawrence Livermore National Laboratory and the Vulcan laser at the Rutherford Appleton Laboratory) and at the Linac Coherent Light Source (LCLS) free electron laser operating in Stanford (CA), but also discuss future applications. We will focus our discussion on the following examples: 1) Equation of state of carbon near the melting point and electron-ion equilibration pathways[1,2]; 2) Laboratory analogues of carbon white dwarf envelopes close to crystallization[3]; 3) Ion-acoustic dynamics in strongly coupled matter and estimates of transport coefficients.

*g.gregori1@physics.ox.ac.uk

[1] A. Pelka et al. Ultrafast Melting of Carbon Induced by Intense Proton Beams. *Phys. Rev. Lett.*, 105:265701, 2010.

[2] T. G. White et al. Observation of Inhibited Electron-Ion Coupling in Strongly Heated Graphite. *Nature Sci. Rep*., 2:889, 2012.

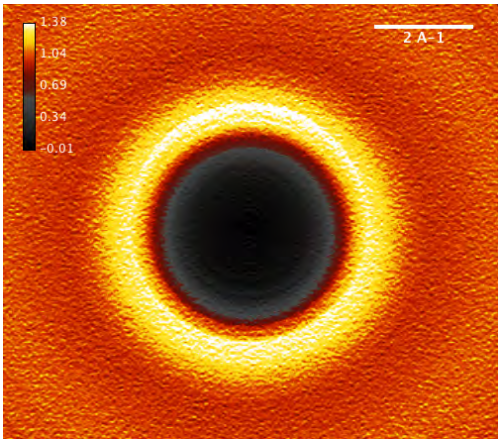
[3] C. R D. Brown et al. Evidence for a Glassy State in Strongly Driven Carbon. *Nature Sci. Rep*., 4:5214, 2014.

Self-organization in dense plasmas: the Gamma-plateau

Jean Clerouin*, P. Arnault, G. Robert
CEA/DAM/DIF, Bruyeres-le-Chatel
91297 Arpajon Cedex France

C. Ticknor, J. D. Kress and L. Collins
Theoretical Division, Los Alamos National Laboratory
Los Alamos, New Mexico 87545, USA

When heated at constant volume (isochoric heating) dense plasmas (10-5000 eV, 1-50 g/cm^3) exhibit the same persistent microscopic structure (same static structure factor) over a wide range of temperatures [1]. In this steady-state regime, which depends on the chosen density and on the atomic number, the ionic thermal motion is essentially independent of the temperature and results in the subtle balance between ionization and temperature. This behavior, suggested by recent simulations, is confirmed by an analysis in the framework of the Thomas-Fermi scaling laws and was indirectly predicted years ago by I. P. Raizer and later by R. M. More. A simple analytical model is derived allowing for the prediction of this self-organized regime: the Γ-plateau [2]. This regime could be used to obtain well-defined experimental conditions in electron heated isochoric experiments on buried layers.
Work performed under the NNSA/DAM collaboration P184.



Simulated diffraction pattern of an tungsten plasma at 40 g/cm^3 and 400 eV. The coupling parameter Γ is about 20. The figure remains the same between 60 to 1200 eV.

jean.clerouin@cea.fr
[1] J. Clérouin, P. Arnault et al., Phys. Rev. E 87, 061101, (2013).
[2] P. Arnault, J. Clérouin et al., Phys. Rev. E 88, 063106 (2013).

Static and dynamic structure factors for warm dense matter

Kai-Uwe Plagemann*[1], Hannes Rüter[1], Thomas Bornath[1], Carsten Fortmann[2],
Michael P. Desjarlais[3], and Ronald Redmer[1]
[1] University of Rostock, Institute of Physics, 18051 Rostock, Germany
[2] QuantumWise A/S, 2100 Copenhagen, Denmark
[3] Sandia National Laboratory, Albuquerque, NM 87158-1186, USA

Warm dense matter of solid-like densities and temperatures of several eV is relevant for planetary interiors and inertial confinement fusion experiments. A versatile and reliable tool to probe such extreme states of matter is X-ray Thomson scattering (XRTS) from which information about plasma parameters like electron density, electron temperature and mean ionization state can be inferred directly from the dynamic structure factor [1]. Pioneering XRTS experiments were performed for beryllium [2,3] and later also for other materials such as boron, carbon and aluminum.

The evaluation of the X-ray scattering spectra is usually based on the Chihara formula [4] that accounts for electronic free-free, bound-free, and bound-bound transitions. We present results for the static and dynamic structure factor based on *ab initio* molecular dynamics simulations. First, the static ion-ion and electron-ion structure factors, which are relevant for the description of elastic scattering of X-rays (ion feature), are calculated from simulation data. We determine the slope of the screening cloud around the ions and compare with analytical expressions [4] that have been used so far. Second, we calculate the dynamic ion-ion structure factor via the time-dependent intermediate scattering function, for the first time using a full Kohn-Sham DFT schema [5]. We compare our results with XRTS experiments for Be and Al. Third, the dynamic electron-electron structure factor is derived in linear response theory using the fluctuation-dissipation theorem and the Kubo-Greenwood formula for the dynamic conductivity. We observe an almost perfect Drude-like for Be [6].

*kai-uwe.plagemann2@uni-rostock.de

[1] S. H. Glenzer and R. Redmer, Rev. Mod. Phys., 81:1625, 2009.

[2] S. H. Glenzer et al., Phys. Rev. Lett., 98:065002, 2007.

[3] H. J. Lee et al., Phys. Rev. Lett., 102:115001, 2009.

[4] J. Chihara, J. Phys.: Condens. Matter, 12:231, 2000.

[5] H. Rüter and R. Redmer, Phys. Rev. Lett., 112, 2014.

[6] K.-U. Plagemann et al., New J. Phys., 14:055020, 2012.

Two-temperature WDM of Al and Au: (quasi)thermodynamics and conductivity

P.A. Zhilyaev and V.V. Stegailov*
Joint Institute for High Temperatures of Russian Academy of Sciences
Moscow, 125412, Russia

Warm dense matter can be attributed to the state of matter at near-solid densities and temperature between 1 eV and 100 eV. Theoretical modeling of WDM is extremely difficult due to electron degeneracy and strong ion-ion coupling. Nevertheless a large number of studies showed that density functional theory (DFT) can be successfully applied to simulate characteristics of WDM. Modelling and simulation of laser interaction with the metal targets deploy the two-temperature approximation [1]. These simulations require data on the (quasi)thermodynamic properties of the two-temperature WDM and its transport properties (thermal conductivity), which depend both on the electron temperature and the ions temperature [2,3]. In this talk I will present our results on the DFT calculations of the EoS and electrical and thermal conductivity of solid and liquid aluminum and gold in the two-temperature states.

*stegailov@gmail.com

[1] G.E. Norman, S.V. Starikov, V.V. Stegailov, V.E. Fortov et al. Nanomodification of gold surface by picosecond soft x-ray laser pulse, *J. App. Phys*, **112**, 013104 (2012)

[2] G.E. Norman, S.V. Starikov, V.V. Stegailov, I.M. Saitov, P.A. Zhilyaev Atomistic modeling of warm dense matter in the two-temperature state, *Contributions to Plasma Physics*, **53**, 129-139 (2013)

[3] G.E. Norman, I.M. Saitov, V.V. Stegailov, P.A. Zhilyaev Atomistic Modelling and Simulation of Warm Dense Matter. Conductivity and Reflectivity, *Contributions to Plasma Physics*, **53**, 300-310 (2013)

Quantum dipolar gases

J. Boronat*
Departament de Física i Enginyeria Nuclear, Universitat Politècnica de Catalunya
Barcelona, Spain

In this talk, I will report on recent results for the many-body physics of dipolar gases obtained in our group using quantum Monte Carlo (QMC) methods. I will show results on a bilayer composed by dipoles with a moment perpendicular to the plane. When the interlayer distance is small enough, up and down dipoles form bound states that break when this distance increases. We observe a transition between a regime of pair superfluidity and another one with only single-particle Bose-Einstein condensation. This offers a unique opportunity to observe pair superfluidity of bosons in the continuum, without an external optical lattice. In the second part, I will show as the anisotropy of the interaction induces the formation of a stripe phase in a system of tilted dipoles in a plane. Using QMC we have been able to determine the phase diagram of planar tilted dipoles as a function of both density and polarization angle, showing the stability limits of the new quantum stripe phase.

*jordi.boronat@upc.edu

Electron oscillations in nonideal cluster nanoplasmas

R.G. Bystryi*, I.V. Morozov

Joint Institute for High Temperatures of RAS, Izhorskaya, 13, build. 2, Moscow 125412, Russia;

Moscow Institute for Physics and Technology, Institutskii per., 9, Dolgoprudny 141700, Russia;

Higher School of Economics, Myasnitskaya, 20, Moscow 101000, Russia

Irradiation of nanosized metallic clusters by femtosecond laser pulses of moderate intensities 10^{13} – 10^{16} W/cm^2 has been considered recently in both experiments and computer simulations[1]. It has been shown that the plasma generated by ionization of cluster atoms is nonideal which allows one to apply these studies to the development of nonideal plasma theory. Electron plasma oscillations, electron-ion collisions, relaxation rates in such plasma are of particular interest in view the size effects essential for clusters[2,3].

The method of molecular dynamics (MD) is one of the most suitable numerical techniques to study dynamical processes in the cluster plasma due to a small number of particles. In this work we propose to use the Graphics Processing Units (GPUs) to accelerate MD simulations of the nonideal plasma. Contemporary GPUs are widely used for scientific computing and showed their high efficiency for a particular class of atomistic simulations[4]. In our case it results in a performance gain up to two orders of magnitude when comparing the contemporary GPU and CPU cores. It allows us to increase the number of particles and observe the transition of the electron oscillation spectra in the cluster plasma ranging from 55 to 10^5 ions.

Using the GPU-accelerated MD simulation code the frequencies and damping of different collective plasma oscillation modes including surface and volume plasmons (Mie and Langmuir oscillations) are studied. Dependence of the electron oscillation spectra on the choice of the interaction potential, the shape and crystallographic group of ionic structure clusters are presented.

*broman.meld@gmail.com

[1] J.A. Anderson, C.D. Lorenz, A Travesset. General purpose molecular dynamics simulations fully implemented on graphics processing units. *Journal of Computational Physics*, 227:5342, 2008.

[2] M. Belkacem, F. Megi, P.-G. Reinhard, E. Suraud, G. Zwicknagel Coulomb explosion of simple metal clusters in intense laser fields. *Physical Review A*, 73:051201, 2006.

[3] T. Raitza, H. Reinholz, G. Repke, I. Morozov, E. Suraud. Laser excited expanding small clusters: Single time distribution functions. *Contributions to Plasma Physics.* 49:496, 2009.

[4] I.V. Morozov, A.M. Kazennov, R.G. Bystryi, G.E. Norman, V.V. Pisarev, V.V. Stegailov. Molecular dynamics simulations of the relaxation processes in the condensed matter on GPUs. *Computer Physics Communications*. 182:1974, 2011.

Using higher ionization states to increase the strong coupling of an ultracold neutral plasma

M. Lyon* and S. D. Bergeson
Brigham Young University
Provo, UT 84602, U.S.A.

We report measurements of an increase in the ion strong coupling of an ultracold neutral Ca^{2+} plasma. Ultracold neutral plasmas are generated by photoionizing laser-cooled atoms close to threshold. The ion strong coupling at early times after the plasma is created is high, due to the very low initial temperature (~1 mK) of the ions. However the strong coupling parameter Γ is limited at times later than ~100 ns by an ultrafast, nonequilibrium relaxation of the ions. This process is called "disorder-induced heating" and it limits Γ in our plasmas to order unity [1]. A recent simulation predicted that higher values of the strong coupling parameter in ultracold neutral plasmas can be realized if the plasma ions are excited to higher ionization states [2]. The maximum value of Γ depends on the time at which the second ionization laser pulses arrive. We have built an experiment in laser-cooled calcium designed to test this prediction and increase the strong coupling of an ultracold neutral plasma by promoting the plasma ions to the second ionization state. Using laser-induced fluorescence we map out the ion velocity distribution of the singly ionized Ca in order to measure the effect that the second ionization has on the temperature of the Ca^+ ions as a function of the second ionization fraction.
*mary_lyon@byu.edu

[1] S. D. Bergeson, A. Denning, M. Lyon, and F. Robicheaux, *Density and temperature scaling of disorder-induced heating in ultracold plasmas.* Phys. Rev. A **83** 023409, (2011).

[2] M. S. Murillo, *Ultrafast dynamics of neutral, ultracold plasmas.* Physics of Plasmas, **14** 055702, (2007).

Collective Excitations in Magnetized Strongly Coupled Plasmas

H. Kählert[1,2*], T. Ott[1], A. Reynolds[2], M. Bonitz[1], G. J. Kalman[3], and H. Löwen[4]

[1)] Christian-Albrechts-Universität zu Kiel, Germany

[2)] University of Birmingham, UK

[3)] Boston College, USA

[4)] Heinrich-Heine Universität Düsseldorf, Germany

The properties of strongly coupled plasmas, such as diffusion or viscosity, change dramatically in the presence of an external magnetic field. In this talk, we present a comprehensive analysis of the wave spectrum of the magnetized strongly coupled one-component plasma by combining the results of first-principle molecular dynamics simulations with a theoretical analysis based on the Quasi-Localized Charge Approximation [1, 2]. This allows us to obtain a comprehensive understanding of the various waves and their interplay, which leads, e.g., to the appearance of higher harmonics.

Complex plasmas are ideally suited to study strongly coupled plasmas in the laboratory. While the ions can be magnetized with the help of superconducting magnets, the magnetization of the heavy dust particles is far more difficult. We present a method that allows one to study strong magnetization and strong coupling effects in a dusty plasma simultaneously [3,4]. It is based on the mathematical equivalence of the Coriolis force in a rotating reference frame and the Lorentz force on a charged particle in a magnetic field. The efficiency of the concept has been proven experimentally for finite two-dimensional clusters [3] as well as extended macroscopic dust layers [5].

This work was supported by the DAAD via a postdoctoral fellowship and the RISE program, the DFG via SFB-TR6 and SFB-TR24, a grant for CPU time at the North-German Supercomputing Alliance HLRN, and NSF grants PHY-0715227, PHY-1105005, PHY-0813153.

*kaehlert@theo-physik.uni-kiel.de

[1] T. Ott, H. Kählert, A. Reynolds, and M. Bonitz, Phys. Rev. Lett. **108**, 255002 (2012)

[2] H. Kählert, T. Ott, A. Reynolds, G. J. Kalman, and M. Bonitz, Phys. Plasmas **20**, 057301 (2013)

[3] H. Kählert, J. Carstensen, M. Bonitz, H. Löwen, F. Greiner, and A. Piel, Phys. Rev. Lett. **109**, 155003 (2012)

[4] M. Bonitz, H. Kählert, T. Ott, and H. Löwen, Plasma Sources Sci. Technol. **22**, 015007 (2013)

[5] P. Hartmann, Z. Donkó, T. Ott, H. Kählert, and M. Bonitz, Phys. Rev. Lett. **111**, 15502 (2013)

Charge-Charge Sum Rules in Near Critical Electrolytes

Subir K. Das[a], Young C. Kim[b] and Michael E. Fisher[c]
[a]Theoretical Sciences Unit, Jawaharlal Nehru Center for Advanced Scientific Research, Jakkur P.O., Bangalore 560064, India
[b]Center for Computational Materials Science, Naval Research Laboratory, Washington, DC 20375, USA
[c]Institute for Physical Science and Technology, University of Maryland, College Park, Maryland 20742, USA

The charge-charge structure factor in a neutral electrolyte solution obeys $S_{ZZ}(k;T,\rho) = \xi_{Z,1}^2 k^2 - \xi_{Z,2}^4 k^4 + ...$, where T and ρ are the temperature and overall ion density while $\xi_{Z,1}$ and $\xi_{Z,2}$ are the second and fourth moment charge-charge correlation lengths. The first and second Stillinger-Lovett [1] charge-charge sum rules state $S_{ZZ}(0;T,\rho) = 0$, referring to electroneutrality, and $\xi_{Z,1} = \xi_D$, where ξ_D is the Debye screening length. From grandcanonical Monte Carlo simulations of a fully size- and charge-symmetric electrically neutral hard-sphere electrolyte, the restricted primitive model, we present results [2] for $\xi_{Z,1}$ and $\xi_{Z,2}$. At the critical point these contradict the generalized Debye-Hückel theory (GDHT) [3] and the exactly soluble charge-symmetric spherical models (CSSM) [4] which support the second sum rule. Since the derivation of the second rule assumes perfect screening of all charges, this finding questions the conducting nature of an electrolyte at criticality. Furthermore, our analysis shows that $\xi_{Z,2}^4$ diverges like the compressibility as one approaches the critical point, again contradicting the GDHT and CSSM that predict finiteness of the fourth moment. On the other hand, the observed behavior is similar to the predictions of the charge-asymmetric spherical models [4].

References:
1. F. Stillinger and R. Lovett, J. Chem. Phys. **48**, 3858 (1968).
2. S.K. Das, Y.C. Kim and M.E. Fisher, Phys. Rev. Lett. **107**, 215701 (2011); J. Chem. Phys. **137**, 074902 (2012).
3. B.P. Lee and M.E. Fisher, Phys. Rev. Lett. **76**, 2906 (1996); Europhys. Lett. **39**, 611 (1997).
4. J.-N. Aqua and M.E. Fisher, Phys. Rev. Lett. **92**, 135702 (2004); J. Phys. A **37**, L241 (2004).

Multiscale Simulation of Dust Clusters in a Strongly Magnetized Flowing Plasma

P. Ludwig*[1], H. Kählert[1], J.P. Joost[1], C. Arran[2], Zh. Moldabekov[3] and M. Bonitz[1]

[1]Christian-Albrechts-Universitt zu Kiel, Germany

[2]Emmanuel College, Cambridge, UK

[3]Al-Farabi Kazakh National University, Kazakhstan

A key problem in the description of non-ideal, multi-component plasmas is the drastic difference in the characteristic length and time scales of the different particle species. This challenging multi-scale problem inherent to studying streaming complex plasmas can efficiently be tackled by a statistical, linear-response ansatz for the light plasma constituents in combination with first-principle Langevin dynamics simulations of the heavy and strongly correlated dust component [1]. Of crucial importance in this scheme is the quality of the dynamically screened Coulomb potential [2,3]. Using the dielectric function for a partially ionized flowing magnetized plasma results are presented for the wakefield around a single dust grain and for multiscale simulations of a correlated ensemble of grains revealing fundamental structural changes when wake effects and an external magnetic field come into play.

This work is supported by the DFG via SFB-TR24, projects A7 and A9 and by the DAAD RISE program.

*ludwig@theo-physik.uni-kiel.de

[1] P. Ludwig, H. Kählert, and M. Bonitz, *Ion-Streaming Induced Order Transition in 3D Dust Clusters*, PPCF **54**, 045011 (2012),

[2] P. Ludwig, W.J. Miloch, H. Kählert, and M. Bonitz, *On the Wake Structure in Streaming Complex Plasmas*, New J. Phys. **14**, 053016 (2012)

[3] P. Ludwig, C. Arran, and M. Bonitz, "Introduction to Streaming Complex Plasmas B: Theoretical Description of Wake Effects", in: "Complex Plasmas: Scientific Challenges and Technological Opportunities", M. Bonitz, K. Becker, J. Lopez and H. Thomsen [eds.], Springer (2014)

Template controlled crystal growth in strongly coupled Coulomb plasma

E. Allahyarov[1,2,3]*, H. Löwen[1], and A. Ivlev[4]

[1] Institut für Theoretische Physik II, HHU Düsseldorf, Germany

[2] Theoretical Department, OIVT RAN, Russian Academy of Sciences, Moscow, Russia

[3] Macromolecular Science, Case Western Reserve University, Cleveland, USA

[4] Max-Planck-Institute for Extraterrestrial Physics, Garching, Germany

The role of damping in the growth of crystalline layers in strongly coupled Coulomb (dusty) plasma is investigated. It is shown that the rate of absorption of the latent heat at the liquid-solid interface strongly affects the propagation velocity and the interface width of the nucleation front. At low damping the accumulation of the latent heat at the nucleation front slows down the propagation of the front and leads to the generation of standing waves in the plasma. We found that a mismatch between the template and bulk particle densities can serve as an effective control parameter both for the direction and for the type of the crystal growth. Particularly, in cases when the template density is much smaller than the density of particles in the bulk, a FCC type crystal growth is detected for the system in the BCC ground state. When put under gravity, more complex nucleation scenarios are detected.

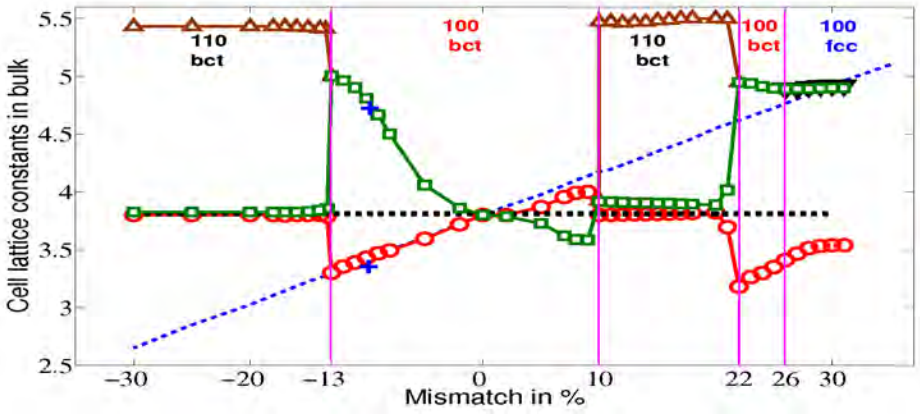


Figure 1: Bulk and template BCC lattice constants for the mismatches ranging from -35% to +35%. Template is 100-oriented BCC lattice parallel to the plane surface. Red line/circles and green line/squares are for the a_x and c_z constants of the BCC cell in the bulk correspondingly. Blue/dashed line is for the template BCC.

*exa54@case.edu

Thursday Talks

How does the cold dusty plasma liquid crack and heal under shear stress?

Chi Yang* and Lin I
Department of Physics and Center for Complex Systems, National Central University
Jhongli, Taiwan 32001, Republic of China

A cold liquid around freezing is no longer fully disordered microscopically. The interplay of strong mutual coupling and weak thermal agitation leads to the heterogeneous structure with solid-like crystalline ordered domains coexisting with defect clusters around domain boundaries. The recent study indicated that the micro-structure can be rearranged through stick-slip type cooperative motion, such as domain crackling, rotation, drift, and healing under weak thermal excitation[1]. How the cold liquid responses microscopically to the additional external stress, from the view of micro-cracking, is a challenging unexplored issue. In this work, this issue is addressed experimentally in a cold dusty plasma liquid[2] composed of negatively charged dust particles suspended in a low pressure rf discharge. A laser beam passing through the center of the liquid is used to generate the shear stress. Dust particle trajectories are directly tracked through video microscopy. Bond dynamic analysis[1] is used to analyze the domain rotating and bond breaking in the structural rearrangement process. Under the weak shear stress comparable with thermal agitation, the crystalline order domains are able to temporally sustain the weak stress and propagate it to remote regions for thermal assisted cracking and structural rearrangement. No preferred regions for crack initiation are observed. On the contrary, the strong shear stress induces higher crack initiation rate in the stress loading zone. The spatiotemporal evolution of the micro-crack propagation and the induced cooperative particle motion are discussed.

*aztme@hotmail.com

[1] Chi Yang, Chong Wai Io and Lin I, Phys.Rev.Lett. 109, 225003 (2012)
[2] Yen-Shuo Su, Chong-Wai Io, and Lin I, Phys.Rev.E. 86, 016405 (2012)

Polarization and finite size effects in correlation functions of dusty plasmas

A. E. Davletov*, L.T. Yerimbetova, A. K. Ospanova and Ye.S. Mukhametkarimov
Department of Physics and Technics, Al-Farabi Kazakh National University
Al-Farabi av. 71, Almaty 050040, Kazakhstan

A pseudopotential model of the dust particles interaction has been recently proposed in [1] to take into account the polarization, finite size and screening effects. The derivation starts from the assumption that the dust particles are made of a conductive material such that their mutual interaction and interaction with the electrons and ions of the buffer plasma can analytically be treated within the method of image charges [2]. Then, the renormalization theory of plasma particles interaction [3], leading to the so-called generalized Poisson-Boltzmann equation, is applied to obtain the interaction potential of two isolated dust grains immersed into the buffer plasma of electrons and ions. The pseudopotential model, developed in such a way, naturally includes the polarization phenomena and the screening due to the buffer plasma and, at the same time, omits the dust number density which fully justifies its further application in various theoretical approaches and computer simulations to treat collective events.

In particular, the above mentioned pseudopotential model is used in the generalized Poisson-Boltzmann equation for the dust component which results in a rather neat analytical expression for the static structure factor of the dust component. Of course, such an approach is only valid for weakly coupled regime and, really, the static structure factor, being monotonic in quite a broad range of plasma parameters, reveals no sign of order formation.

To go beyond the validity range of the proposed analytical expression, the Ornstein-Zernike relation in the hyper-netted chain approximation (HNC) is numerically solved to obtain the static structure factor of the dust grains whose non-monotonic behavior clearly indicates the short- or even long-range order formation in a specified plasma parameters domain.

Finally, the Monte-Carlo simulation has been conducted and its results for the radial distribution function of the dust particles are checked against the solution of the HNC equation to find quite a good agreement for sufficiently large values of the dust coupling parameter.

*askar@physics.kz

[1] L. T. Erimbetova, A. E. Davletov, Zh. A. Kudyshev, and Ye. S. Mukhametkarimov. *Influence of Polarization Phenomena on Radial Distribution Function of Dust Particles.* Contrib. Plasma Phys., **53** 414, (2013).

[2] V. A. Saranin, and V. V. Mayer. *Interaction of Two Charged Conducting Balls: Theory and Experiment.* Phys. Usp., **53** 1067, (2010).

[3] Yu. V. Arkhipov, F. B. Baimbetov, and A. E. Davletov. *Self-consistent Chemical Model of Partially Ionized Plasmas.* Phys. Rev. E, **83** 016405, (2011).

Strongly Coupled Complex Plasmas: Effective Potentials and Physical Properties

T. S. Ramazanov*
IETP, Al-Farabi Kazakh National University
Almaty, 050040, Kazakhstan

Microscopic, thermodynamic and dynamical properties of a strongly coupled complex plasma are studied by theoretical and experimental methods. In order to describe the interactions between particles several effective potentials are used. These potentials take into account quantum mechanical, screening and polarizations effects in nonideal [1] and complex [2] plasmas. The effective potentials between dusty particles in plasma are derived on the basis of the method of dielectric response functions. The grains are considered as dipoles due to the nonequilibrium effects in dusty plasma. As a result, the dipole-dipole effective interaction potentials are obtained for several cases. It is shown that the calculated effective potentials have an oscillating character and depend on plasma parameters.

The Coulomb logarithm for a dense semiclassical fully and partially ionized plasma was derived. Stopping power and relaxation processes of nonideal plasma were studied on the basis of the Coulomb logarithm [1,4]. The comparison with data of other theoretical and experimental works was carried out.

Two methods for diagnostics of dusty plasma parameters are proposed [3,5]. Firstly, we use the dependence between microscopic and macroscopic properties of the system. In order to determine the plasma parameters the sum rules and normalization relations were used. In the second case a new method for determination of the buffer plasma parameters was developed by measuring of the dust-free region area around the Longmuir probe. The experimental results were compared with the data of theoretical study on the basis of the balance equation of the dust particles thermal energy and their electrostatic interaction energy with the probe.

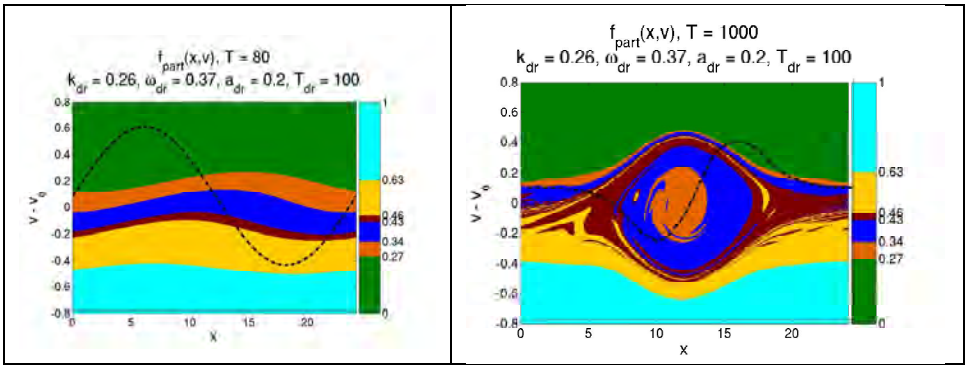
*ramazan@physics.kz

[1] T.S. Ramazanov, S.K. Kodanova, Zh.A. Moldabekov and M.R.Issanova. Dynamical properties of non-ideal plasma on the basis of effective potentials. *Phys*. *Plasmas*, **20,** 112702 (2013)
[2] T.S. Ramazanov, Zh.A. Moldabekov, K.N. Dzhumagulova and M.M. Muratov. Pseudopotentials of the particles interactions in complex plasmas. *Phys*. *Plasmas*, **18,** 103705 (2011).
[3] Y.A.Ussenov, T.S.Ramazanov, K.N.Dzhumagulova and M. K. Dosbolayev. Application of dust grains and Langmuir probe for plasma diagnostics. *Europhys*.*Letters*, **105,** 15002 (2014)
[4] T. S. Ramazanov, Zh. A. Moldabekov, M. T. Gabdullin, and T. N. Ismagambetova. Interaction potentials and thermodynamic properties of two component semiclassical plasma. *Phys*. *Plasmas*, **21,** 012706 (2014)
[5] S.A.Orazbayev, M.M.Muratov, T.S.Ramazanov, M.K.Dosbolayev, M.Silamiya, M.N.Jumagulov, and L. Boufendi. The Diagnostics of Dusty Plasma in RF Discharge by Two Different Methods. *Contr*. *Plasma Phys*., **53,** 436 (2013)

Nonlinear Kinetic Self-Organized Asymptotic States in High Energy Density Plasmas: Pump-Probe df/dv Diagnostics from the Visible to X-Rays

Bedros Afeyan,
Polymath Research Inc.
Pleasanton, CA 94566, U.S.A.

We will describe nonlinear, nonstationary, self-organized asymptotic kinetic states in high energy density plasmas. An example is KEEN (kinetic electrostatic electron nonlinear) waves [1]. Where trapping-untrapping and nonlocal retrapping oscillations give rise to multiple-harmonic, phase locked, coherent electric fields despite chaotic particle orbits and nonadiabatic separatrix crossings. We will discuss how such states may be generated and how they may be diagnosed in the laboratory using pump-probe optical mixing techniques. STUD (Spike Trains of Uneven Duration and Delay) pulses [2] on the pump and ultrafast diagnostics on the probe are two of the requirements for the fulfillment of the new diagnostics system. From visible to X-ray regimes will be considered. The goal is to control laser-plasma instabilities such as stimulated Raman and Brillouin scattering by modulating the pump laser on and off on a ps time scale. Diagnosing the resulting growth spurts of the probe indicates the evolution of the electron and ion distribution functions on a ps time scale and with very small (beam crossing volume) spatial resolution as well. The plasma may be undergoing violent instabilities but the optical mixing technique will tame the results of the diagnostics system itself. Then, gain in the transient regime allows one to recover the Landau damping rate changes, which are in turn proportional to changes to the slope of velocity distribution functions. Kinetic and fluid simulation results will be shown and future prospects of performing such experiments on Trident at LANL and on MEC at LCLS, SLAC.



*bafeyan@gmail.com

[1] B. Afeyan et al., KEEN Waves, http://arxiv.org/abs/1210.8105 , http://arxiv.org/abs/1211.1437
[2] B. Afeyan et al., STUD pulses, http://arxiv.org/abs/1210.4462, http://arxiv.org/abs/1304.3960

Method of separation of polydisperse particles in plasma of radio–frequency discharge

D. Batryshev[1,2,*], T. Ramazanov[1,2], M. Dosbolayev[1,2], M. Gabdullin[1,2], S. Orazbayev[1]
[1]Institute of experimental and theoretical physics, Al-Farabi Kazakh National University, 71, al-Farabi av., Almaty,050040,Kazakhstan
[2] National nanotechnological laboratory of open type, Al-Farabi Kazakh National University,71, al-Farabi av., Almaty, 050040, Kazakhstan

Monodisperse particles are particles which have the same geometrical parameters or phase states. For a strictly monodisperse system, the size distribution curve for such a system is represented by a narrow peak of Gaussian distribution.

In this paper the method of polydisperse particles separation in plasma of radio-frequency discharge for obtaining of monodisperse particles are considered. Difference of proposed method from other one is external influence absence of impurity, because the separation process goes in a plasma reactor, also it is possible to use a different kind of materials for separation [1]. Mechanism of this method based on using a special form of plasma (electric) field, which allows to select and collect dusty particles by mass from crystal-like structure of dusty plasma. A condition for obtaining monodisperse particles is spherical form of particles, in other cases we can only speak about the smallness dispersions of separated particles.The experimental setup was described in detail in previous works [2].

The experiment was carried out in argon plasma at constant pressure of argon gas 0.3 Torr and different power of discharge. For separation polydisperse spherical particles of glass (SiO_2) with diameters 1 – 100 μmhave been used. After separation obtained particles had diameters 5 μm. Range of separation is 600 nm - 50 μm.

*batryshev@physics.kz

[1] V. Gente, F.L. Marca, F. Lucci, P. Massacci, Waste Management 23, 951–958 (2003)
[2] Dosbolayev M.K., Utegenov A.U., Ramazanov T.S., Daniyarov T.T. Structural and transport properties of dust formation in plasma of noble gases mixture in RF discharge // Contrib. PlasmaPhys. – 2013. – V. 53, №. 4-5. – P. 426-431.

A Non-Born-Oppenheimer Molecular Dynamics Method for Dense Plasmas

David Michta[1,*], Liam G. Stanton[1], Mike Surh[1], Frank Graziani[1] and Michael S. Murillo[2]
[1]Lawrence Livermore National Laboratory, [2]Los Alamos National Laboratory

Most molecular dynamics methods assume either a pair ionic potential, in which the electrons only appear indirectly, or obtain ionic forces from the total electron density, which effectively incorporates *N*-body forces. The latter category, often referred to as "*ab initio*" or "quantum" molecular dynamics, represents an extremely accurate method that has been implemented in various software packages, such as Quantum Espresso [1], Abinit, and VASP, and is most often built upon a Born-Oppenheimer, plane-wave, pseudopotential electronic structure method. However, for several important problems in dense plasmas these assumptions are not appropriate and an alternate computational method is needed. In particular, we desire a method that treats the electrons dynamically, quantum mechanically, with no assumptions about the bound/core states, and efficient computationally. We have developed such a method by combining the usual molecular dynamics methods for the ions with an electron fluid model based on an all-electron, time-dependent, orbital-free density functional theory (OF-DFT) approach. In our method, we solve the coupled time-dependent equations of motion of the ions and the density and momentum equations for the electron fluid, a form of quantum hydrodynamics. Our momentum equation has been constructed to yield a desired OF-DFT thermodynamic ground state in equilibrium, thereby guaranteeing high-quality equation of state properties. For example, with the use of a long-wavelength (Thomas-Fermi) functional, we are able to approximately describe non-equilibrium dense plasmas over many orders of magnitude variation in temperature. We have analyzed this model theoretically to understand its physical properties, and we will discuss those predictions, which range from collective modes (electron plasma waves, ion-acoustic waves, *etc*.) to density fluctuations (dynamic structure factor, *etc*.). We have also implemented numerical methods based on implicit time stepping and finite volume. These methods produce a fast numerical scheme with good conservation properties and are second order accurate. We will present numerical results for the density fluctuations, including wave dispersion relations, that reveal the non-Born Oppenheimer (NBO) dynamics for a range of temperatures from T = 0 to T = 1keV. Next, we apply the method to the important problem of charged particle stopping. We examine the case of a high-Z projectile [2] in warm dense matter, which provides a stringent test of NBO physics, since the projectile creates a non-linear wake potential in the dynamic electrons, and the number of "bound" electrons is velocity dependent and not known *a priori*. Finally, we end with an outlook toward future developments in numerical methods, improved OF-DFT models, and various applications.

Figure 1: Fast particles require a NBO treatment. Here, a fast proton traverses warm dense matter.

[1] P. Giannozzi et al., *J. of Phys.: Condensed Matter* **21**, 395502 (2009).
[2] S. K. Sharma et al., *Applied Radiation and Isotopes* **46**, 39 (1995); G. Cesini and G. Lucarni, *Nucl. Intr. and Methods* **127**, 570 (1975); N. Bohr, *Phys. Rev.* **59**, 270 (1941).

Registration of clots images of dense plasma in the hard X-ray range

*[1]Pavlov G.A., [2]Suslov N.A.,[3]Treushnikov V.M, [2]Garanin P.V., [2]Pozdnyakov Y.V,
[3] Treushnikov V.V., [2]Zhidkov N.V.

[1]IPCP RAS, Chernogolovka, Moscow region, 142432, Russia
[2]RFNC-VNIIEF, ILPI, Sarov, Russia
[3]PC "Reper-NN", Nizhny Novgorod, 603003, Russia

The research of the thermophysical properties of plasma in extreme states is important both in principle and for different applications. In experiments on the measurement of these properties, as a rule, were observed their averaged values of plasma formation. To increase the accuracy of experimental data, you must know the degree of homogeneity in the study of plasma clot.

Application of optical methods in the visible range with this purpose, it is often impossible because of the powerful thermal radiation of the plasma, which must be escaped by shield. Therefore, plasma diagnostics is proposed in the hard X-ray range using X-ray polymer refractive lenses with axial symmetry, combined in a compound lens (10-12 single lenses) with the desired characteristics.

To produce refractive lenses we have been developed manufacturing technique of lenses with axial symmetry and a parabolic profile of the cavity using shape memory polymer. These lenses are tested [1] and showed high radiation resistance. Achieved technological advantages enable qualitatively improve a focusing of radiation and resolution of images by the single and compound lenses compared with existing analogues. Other advantages of the shape-memory polymer refractive lenses are cheapness and safe of use. To manufacture X-ray lenses the oligomers of methacryl series have been synthesized and photopolymerizable composition of strictly defined properties developed. The original one-step variant of frontal photopolymerization method is used to get the defect-free products of precisely shape without destructive processes and thermal shrinkage. Lack of defects in the polymer product, in turn, is one of the basic conditions of their abnormally high resistance to various factors, including the hard X-rays. This circumstance gives the maximum possibility to adapt the characteristics of these lenses with the requirements of X-ray optics.

Plasma clot occurred under the action of powerful laser pulse on the copper foil. As a radiation source used iodine laser installation [2]. The energy of the laser pulse was 280 J, pulse duration - 0.40 ns. Radiation with a wavelength of 1 = 1.315 microns focused on the target surface. Spot exposure was determined using a composite X-ray lens and camera-obscura, the resulting image of a bunch of laser plasma in the hard X-ray energy range was 8 Kev. Found the size of the irregularities in the X-ray intensity is determined by the resolution of the combined X-ray lens and the level of 10-20 micron.

Thus, it is shown that the use of composite X-ray lenses proposed design enables to receive local and sufficiently detailed experimental data on dynamics of plasma clots in extreme condition (which study is difficult by optical methods). One can explore the geometrical sizes, the degree of homogeneity, the spectral composition of X-ray radiation, etc of plasma clots. A set of experimental characteristics appropriates to compare with the data of computer modeling of the relevant gas-dynamic processes.

*E-mail: pavl4411@eandex.ru

[1]. G. Pavlov. I. Snigireva, A. Snigirev, T. Sagdullin, M. Schmidt
X-ray spectrometry, V. 41 , P. 313-315, 2012
[2]. Gus'kov S.Yu., Demchenko N.N., Zhidkov N.V. et al
JETP, V.138, No.3(9), P. 524-543, 2010

Collective modes in binary systems: Coulomb vs. Yukawa

G. J. Kalman[1], Z. Donko[1,2], P. Hartmann[1,2], K. I. Golden[3], L. Silvestri[1],
[1]Boston College, Chestnut Hill, MA 02467, USA
[2]Wigner Research Centre for Physics, Budapest, Hungary
[3]University of Vermont, Burlington, VT, USA

The profound difference between the collective mode structures of systems with long range (LR) and short range (SR) interactions is well understood. The plasmon, the hallmark of the LR interaction in a system of charged particles with a neutralizing background, is totally absent in its SR equivalent, a system governed by Yukawa interaction, where the dominant long wavelength excitation is the Goldstone type acoustic phonon. The details of how the transition from the SR type to the LR type excitation occurs as the range of the Yukawa potential goes to infinity, has been elucidated by many researchers [1]. With two different species – a binary ionic mixture- the picture becomes more involved: the plasmon splits into a doublet of high frequency (first) and low frequency (second) plasmons, with the appearance of an additional transverse plasmon [2]. While the plasma frequency for the plasmon is strictly coupling independent (as demanded by the Kohn sum rule), the frequencies of the doublet depend strongly on the coupling strength, to the extent that at weak coupling they merge into one single excitation [2]. For the Yukawa system, it is the surviving acoustic mode that develops a complex coupling dependence, via the formation at strong coupling of a "virtual average atom", which governs the sound speed associated with it [3], [4]. We have studied these scenarios as the system develops through a wide range of coupling values, both analytically with the aid of the Quasi Localized Charge Approximation and through Molecular Dynamics simulations. We also show the details of the transition from the binary SR to the binary LR mode structure as the range is extended to infinity.

Partially supported by NSF and OTKA (Hungary).

*gabor.kalman@bc.edu

[1] P. W. Anderson, Phys. Rev. **130**, 439 (1963).
R. V. Lange, Phys. Rev. Lett**. 14,** 3 (1965).
[2] G. J. Kalman, Z. Donko, P. Hartmann, and K. I. Golden, (2014), arXiv:1403.7810 [physics.plasm-ph].
[3] G. J. Kalman et al., Phys. Rev. E **87**, 043103 (2013).
[4] G. J. Kalman et al., Phys. Rev. Lett. **107**, 175003 (2011)

Molecular Dynamics Simulation with Momentum Dependent Potentials: Comparison of High Order Symplectic Integrators

Gautham Dharuman*, Guclu Yaman, Andrew Christlieb and John Verboncoeur
Michigan State University,
East Lansing, MI 48824, U.S.A.

Michael S. Murillo
Los Alamos National Laboratory
Los Alamos, NM 87545, U.S.A

Strongly coupled plasmas are characterized by collective effects that arise as a result of strong inter-particle interactions. A computational study of this system requires molecular dynamics simulations for a detailed understanding of the processes involved. Classical simulations are feasible but result in instabilities as a result of neglecting quantum effects that play a major role in the system evolution. Electron-ion systems, for example, are prone to the so-called "Coulomb Catastrophe" as a result of the infinitely deep coulomb potential of the ion without any stabilizing effect in a classical treatment. To avoid quantum mechanical simulations, effective quantum potentials that supplement the classical treatment are required. This is possible through momentum dependent pseudo-potentials which accommodate the Heisenberg Uncertainty and Pauli Exclusion principles. This work particularly focuses on one class of such potentials called the Kirschbaum-Wilets potentials[1]. These potentials have found successful applications in quasi-classical studies of atomic processes like strong field ionization, stopping power and particle-capture into Rydberg orbits[2]. Since molecular dynamics simulations involve numerical evolution of particle trajectories over long time scales, it is preferred to use integration schemes that conserve the invariants of motion within certain bounds. This is realized through schemes that are symplectic. With the momentum-dependent potentials, the Hamiltonian is non-separable and requires implicit symplectic schemes[3]. For systems involving several particles, implicit methods can be computationally demanding compared to explicit methods. Therefore, implicit schemes with minimum number of function evaluations for a given acceptable error need to be identified. As the first step, the widely used velocity-Verlet scheme is found to result in energy drift thereby losing its symplectic property for the Hamiltonian under consideration. Further, we compare partitioned and non-partitioned symplectic schemes[2] for errors in the total energy, angular momentum and linear momentum and the corresponding number of function evaluations required. Diagonally and fully implicit Runge-Kutta methods are considered, as well as high order composition methods.

*dharuman@egr.msu.edu

[1] C. L. Kirschbaum and L. Wilets. Classical Many-Body Model for Atomic Collisions Incorporating the Heisenberg and Pauli Principles. *Phys. Rev. A* **21**: 834, 1980.

[2] J. S. Cohen and L. Wilets. Fermion Molecular Dynamics in Atomic, Molecular and Optical Physics. *Contemp. Phys*. **39**:163, 1998.

[3] E. Hairer, C. Lubich and G. Wanner. *Geometric Numerical Integration*. Springer Series in Computational Mathematics, second edition, 2006.

Work supported by Air Force Office of Scientific Research

Electronic transport properties of dense plasma

H. D. Whitley[1],* M. P. Desjarlais[2], C. R. Scullard[1], L. X. Benedict[1], J. I. Castor[1],
M .S. Murillo[3], and F. R. Graziani[1]
[1]Lawrence Livermore National Laboratory
Livermore, CA 94551, U.S.A.
[2]Sandia National Laboratory
Albuquerque, NM 87123, U.S.A.
[3]Los Alamos National Laboratory
Los Alamos, NM 87544, U.S.A.

We have applied the ddcMD molecular dynamics (MD) code to the computation of the electrical conductivity and thermal conductivity of hydrogen plasmas. Quantum mechanical effects on the electronic degrees of freedom are incorporated through the use of temperature-dependent statistical potentials. We find that including an artificial interaction to attempt to mimic the Pauli exclusion principle leads to an unphysical increase in the electron-electron scattering cross section, producing unphysically low values of the thermal conductivity. Our MD results are in good agreement with quantum kinetic theory when the artificial Pauli interaction is not used. Quantum, density functional MD (DFT-MD) also yields electrical conductivities that are in agreement with the quantum kinetic theories. On the other hand, thermal conductivities computed with DFT-MD are discrepantly high. These results motivate the application of a beyond mean-field correction to the electron-electron treatment of DFT-MD for thermal conductivity. Prepared by LLNL under Contract DE-AC52-07NA27344.

*heather@llnl.gov

[1] R.M. More, K.H. Warren, D.A. Young, and G.B. Zimmerman, Phys. Fluids 31, 3059 (1988).

Kinetic approach to the dynamics of inhomogeneous strongly coupled plasmas

H. Kählert[1,2*], G. J. Kalman[2], and M. Bonitz[1]

[1)] Christian-Albrechts-Universität zu Kiel, Germany

[2)] Boston College, USA

Non-neutral plasmas in Penning traps, dusty plasmas trapped in external potentials, or finite-size laser produced plasmas belong to a class of strongly coupled plasmas with possibly very inhomogeneous density distributions, which is the reason why their theoretical description is particularly challenging. We approach the problem by using an extended Singwi-Tosi-Land-Sjölander (STLS) ansatz [1] for the two-particle distribution function in combination with the Bogolyubov-Born-Green-Kirkwood-Yvon hierarchy. From the second equation of the hierarchy we obtain an equation for the time evolution of the pair correlation function, which is coupled to the dynamics of the one-particle distribution [2]. We find that the linear theory is closely related to the Quasi-Localized Charge Approximation [3] but includes additional thermal effects. As an application of the theory, we study the breathing mode of confined dust clusters. Comparison with the standard STLS ansatz shows that the extended ansatz yields significantly improved agreement with molecular dynamics simulations in the strong coupling regime.

This work was supported by the DAAD via a postdoctoral fellowship, the DFG via SFB-TR24, and NSF grants PHY-0715227, PHY-1105005, PHY-0813153.

*kaehlert@theo-physik.uni-kiel.de

[1] K. S. Singwi, M. P. Tosi, R. H. Land, and A. Sjölander, Phys. Rev. **176**, 589 (1968)

[2] H. Kählert, G. J. Kalman, and M. Bonitz, submitted

[3] G. Kalman and K. I. Golden, Phys. Rev. A **41**, 5516 (1990)

Simulation of Confined System of Interacting Fermions by Antisymmetrized Wave Packet Molecular Dynamics

I. A. Valuev*, N.A. Kazeev, I. V. Morozov
Joint Institute for High Temperatures of RAS
Izhorskaya 13 bld 2, Moscow, 125412, Russia

The method of Wave Packet Molecular dynamics [1] is an approximate quantum method for numerical simulation of many-particle dynamics. In this method single electron wave functions are expanded in a set [2] of floating Gaussian wave packets (WP) ϕ_k. The Gaussians are referred to as floating because their parameters (positions, momenta, etc.) are treated as dynamical variables. A trial many-body wave function is then constructed depending on the quantum statistical properties of the simulated ensemble, for example for fermions (electrons) a single Slater determinant antisymmetrized product is usually used for each spin projection. The trial wave function is substituted into the time dependent Schroedinger equation and the resulting equations of motion follow from the variational principle [3]:

$$\frac{dq_i}{dt} = \sum_j (\mathbf{N}^{-1})_{ij} \frac{\partial H}{\partial q_j}, \qquad (1)$$

where {q} is the complete set of all dynamical variables of all WPs, $N_{ij} = -2\hbar \mathrm{Im}\left\langle \frac{\partial \Psi}{\partial q_i} \middle| \frac{\partial \Psi}{\partial q_j} \right\rangle$ is the norm matrix and H is the quantum expectation value of the energy for a given trial wave function. The elements of the Hamiltonian and norm matrices may be obtained analytically, however inversion of the matrix is required at every time step of the numerical integration.

The unlimited broadening of the Gaussian wave packets and underestimation of the electron-electron and electron-ion collision frequencies is known to be the major problems of the WPMD method [4] when applied to many-particle systems with homogeneous density, for example plasma systems. However, as known from earlier works [5], the method is able to excellently describe the thermodynamics of a fermionic system confined in the 1D harmonic potential. In this work we study a system of electrons in a 3D confinement potential constructed from harmonic walls and a flat floor. We analyze the correctness of the thermodynamics predicted by the WPMD method in this confinement by comparing it in the limit of a large number of particles with the known theoretical predictions for the homogenous electron gas. We show that the infinite WP broadening that is directly related to the infinite statistical sum in an unconstrained system does not appear in the confined system. By comparing the difference between the confinement and the previously applied variants of the periodical boundary conditions, we conclude that application of the correct quantum boundary conditions is crucial for the successful plasma simulations with WPMD. Periodical boundary conditions for modeling the homogenous system are possible, but they should not augment the number of allowed quantum states in the system phase space. The effects of the attracting electron-ion interaction on the confined system simulations and applications to the hot dense matter are discussed.

*valuev@ihed.ras.ru

[1] A.A. Frost, *J. Chem. Phys.*, 47:3707 (1967)
[2] I. V. Morozov and I. A. Valuev, *Contrib. Plasma Phys.* 52:140 (2012)
[3] D. Klakow, C. Toepffer, P. G. Reinhard, *J. Chem. Phys.*, 101:10766 (1994).
[4] I.V. Morozov, I. A. Valuev, *J. Phys. A*, 42:214044 (2009).
[5] H. Feldmeier, J. Schnack, *Rev. Modern Phys.*, 72:655 (2000)

Molecular Dynamics simulations of the classical one-component Coulomb plasma over the range $0.05 \leq \Gamma \leq 10000$

I. Korolov[1], G. J. Kalman[2], L. Silvestri[2], Z. Donkó[1,2,*]

[1]Wigner Research Centre for Physics, Budapest, Hungary

[2]Physics Department, Boston College, Chestnut Hill, USA

The One Component Plasma (OCP) model has been playing a distinct role in the field of strongly coupled plasmas. Its prominent properties (thermodynamics, transport, collective excitations, etc.) have been investigated by numerous authors, see e.g. [1]. The increase of computational power now allows simulations with improved statistics and accuracy. We present Molecular Dynamics simulation results for the dynamical structure function, $S(k,\omega)$, over a wide range of the coupling parameter Γ, covering the liquid and solid phases. With increasing coupling we can follow the positive-to-negative transition of the slope of the $\omega(k)$ dispersion curve at small wave numbers caused by the onset of correlations. The good signal-to-noise ratio of the data over several orders of magnitude allows examination both of the high frequency tail of $S(k,\omega)$, and of the $S(k,\omega \to 0)$ behavior. We identify the generation of waves at the higher harmonics of the plasma frequency. Work partially supported by NSF and OTKA.

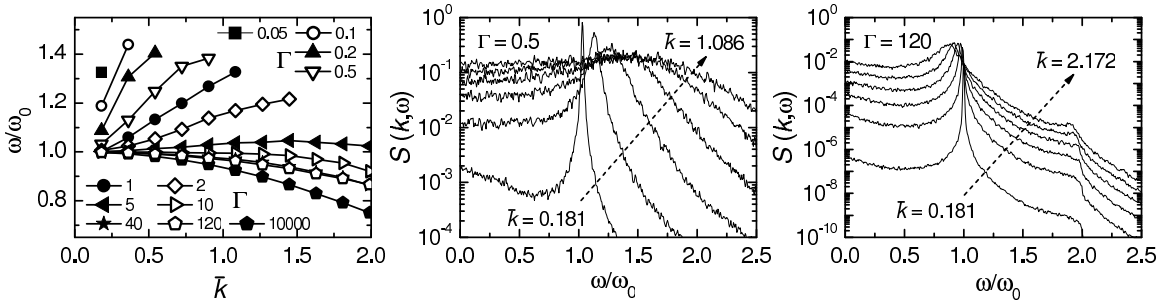


Figure 1: Dispersion relations of the OCP for a wide range of Γ, and examples of $S(k,\omega)$ for a series of wave numbers at $\Gamma = 0.5$ and 120. ω_0 is the plasma frequency, $\bar{k} = ka$, where a is the Wigner-Seitz radius. Note the disappearance of the plasmon mode with increasing $\bar{k}$ at small Γ and the appearance of a second harmonic wave at high Γ. Number of simulation particles: 10,000.

*donko.zoltan@wigner.mta.hu

[1] S. G. Brush, H. L. Sahlin, and E. Teller, J. Chem. Phys. 45, 2102 (1966); J.-P. Hansen, I. R. McDonald, and E. L. Pollock, Phys. Rev. A 11, 1025 (1975); W. L. Slattery, G. D. Doolen, and H. E. DeWitt, Phys. Rev. A 21, 2087 (1980); Z. Donkó, G. J. Kalman, and K. I. Golden, Phys. Rev. Lett. 88, 225001 (2002); J. Daligault, Phys. Rev. Lett. 96, 065003 (2006).

Investigation of dusty plasma properties in various gas mixtures

M.K. Dosbolayev*, T.S. Ramazanov, A.U. Utegenov
Al Farabi Kazakh National University, IETP, al Farabi 71, Almaty, 050040, Kazakhstan.

Properties of dust formations in plasma environment are explored in a large number of experimental and theoretical studies (see reviews [1-2]). Properties of dusty plasma structures are sensible to the conventional experimental parameters: properties of dust particles; composition and properties of buffer gas; and parameters of gas discharge. Investigations of dusty plasma in a mixture of gases is an important factor in the study of the phase transition; in obtaining of new materials in condensed media; for the separation of charged macroparticles in the plasma, etc. Given subjects theoretically were firstly proposed in [3] and experimentally studied in several laboratories in the gas discharge of DC and RF, the results of which are shown in [4-7].
In this paper we present the results of an experimental study of dusty plasma in mixtures of gases in the radio-frequency capacitive discharge. In these experiments the change in the properties of the dusty plasma was investigated in gas mixtures: *Ar+He, Ar+H_2, Ar+CH_4*, as well as in pure gases of *Ar, He, H_2, CH_4*. In particular, comparing the results of experiments which were carried out in pure gases and in mix of gases we studied the influence of the dust formation on dynamic and structural properties. We made a calculation to determine the electron density and temperature based on the method of plasma diagnostics using high-frequency compensated electric probe and spectroscopic method of diagnostics, results of both methods were compared.
Thus, it was found that adding a small amount of relatively heavy gas (in these experiments, *Ar 3-5 %*) to the plasma of light gas (*He, H_2, CH_4*) the properties of plasma dust formations vary considerably [8].

*merlan@physics.kz

[1] H.M. Thomas and G.E. Morfill. 1996, Nature (London) 379, pp 806-809.

[2] V.E. Fortov, A.G. Khrapak, S.A. Khrapak, V.I. Molotkov, O.F. Petrov, 2004. Uspehi Fiz. Nauk (Progress in Physics Sciences.) 174 495 v. - (in Russian) .

[3] S.A. Maiorov, 2007. Short communication on physics FIAN. **7** 44. (in Russian).

[4] S.A. Maiorov, T.S. Ramazanov, K.N. Dzhumagulova, A.N. Jumabekov, and M.K. Dosbolayev, 2008, Phys. Plasmas Vol. 15. P84.

[5] T.S. Ramazanov, T.T. Daniyarov, S.A. Maiorov, S.K. Kodanova, M.K. Dosbolayev and E.B. Zhankarashev, 2011, Contrib. Plasma Phys. Vol. 51, Issue 6, pp 505-508.

[6] M.K. Dosbolayev, T.S. Ramazanov, A.U. Utegenov, T.T. Daniyarov, 2013, Contrib. Plasma Phys. Vol. 53, Issue 4-5, pp 426-431.

[7] S.N. Antipov, M.M. Vasil'ev, S.A. Maiorov, O.F. Petrov, and V.E. Fortov, ISSN 1063-7761, Journal of Experimental and Theoretical Physics, 2011, Vol. 112, No. 3, pp. 482–493.

[8] M.K. Dosbolayev, , A.U. Utegenov, T.S. Ramazanov, R.K. Tentekova, 2014. 7-th International Conference On The Physics Of Dusty Plasmas, New Delhi, India. Book of Abstracts, pp. 70.

Pressure of the Dust Component Due to the Interaction

M. M. Muratov*[1], T.S. Ramazanov[1], K.N. Dzhumagulova[1], J.A. Goree[2]
[1]IETP, al-Farabi Kazakh National University
Almaty, 050040, Kazakhstan
[2] The University of Iowa
Iowa city, Iowa 52242, USA

Dusty plasma is ionized gas which contains particles of condensed matter. These particles, called as dust grains, can have sizes varying from several nanometers to hundreds of microns. Dust grains may have the right sphere shapes or irregular shapes and are made of dielectric or conducting matters. Dusty plasma used to exist in the cosmic plasma, the planetary plasma and in the laboratory plasma.

In this work the thermodynamic properties of dusty plasma were investigated. On the basis of the radial distribution functions dusty plasma's thermodynamic function, such as the excess pressure of the dust component due to the interaction of the charged particles, was evaluated.

Dust grains were considered as particles with dipole moment. For this case the effective interaction potential obtained in work [1] was used. This effective potential was obtained on the basis of the linear dielectric response theory by the random phase approximation. It takes into account the screening effects at large distances:

$$\Phi(r) = \frac{1}{r}\left[Ah(K_1 r) + Bh(K_2 r)\right] + \frac{eZm_{ij}}{r^2}, \tag{1}$$

where h, A, B, K_1 and K_2 are some coefficients.

Two different methods were implemented to obtain radial distribution function for dusty plasma: first one uses experimental data [2], second one uses the exponential approximation:

$$g(r) = \exp(-\Phi(r)/k_B T), \tag{2}$$

where $\Phi(r)$ is the effective interaction potential of the dusty particles (1).

The pressure of the dust component on the basis of the radial distribution functions is expressed by the following relation [3]:

$$P = P_{id} - \frac{n^2}{3}\int_0^{\infty}\int_0^{2\pi} g(r,\theta)\frac{\partial\Phi(r,\theta)}{\partial r} r^3 dr d\theta, \tag{3}$$

where θ is the angle between the dipole moments of two dust grains, P_{id} is the pressure of the ideal gas.

Results were compared with computer simulation data [4] obtained on the basis of the Yukawa interaction potential. Reasonable agreement was shown.

*mukhit.muratov@gmail.com

[1] T.S. Ramazanov, Zh.A. Moldabekov, K.N. Dzhumagulova and M.M. Muratov, *Phys. Plasmas* **18** (2011) 103705.

[2] O.S. Vaulina, O.F. Petrov, V.E. Fortov, A.V. Chernyshev, A.V. Gavrikov, I.A. Shakhanova, and Yu.P. Semenov, *Plasma physics reports* **29 8** (2003), 698-713.

[3] T.S. Ramazanov, K.N. Dzhumagulova et al., Contrib. Plasma Phys. 49, No.1-2, 15-20 (2009)

[4] P.Hartman, G.J. Kalman, Z. Donko, K. Kutasi, *Phys.Rev E* **72** (2005) 026409.

Shock Behavior in Strongly Coupled Dusty Plasmas

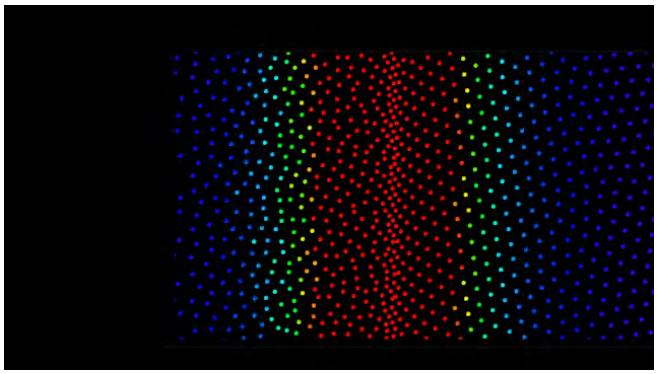
M. Marciante and M. S. Murillo
Computational Physics and Methods Group
Los Alamos National Laboratory
Los Alamos, NM 87545, U.S.A.

Shocks are of wide interest in plasmas because they are a type of non-linear wave propagation, used in measuring equations of state, and act a heating technique. For all of these reasons, a better understanding of shock physics at the microscopic level is needed. In particular, we are interested in phases of matter between solid and plasma, such as strongly coupled plasmas: how does Coulomb coupling impact shock physics? Dusty plasmas provide a unique platform to examine basic shock physics because of the wide range of achievable couplings and because imaging technology allows for detailed measurements at the kinetic level. Recently[1], for example, the Rankine-Hugoniot relations were used to measure the equation of state of a dusty plasma crystal; despite the obvious appearance of a crystal, the surprising result of an *ideal gas* equation of state was inferred.

Here, we use MD to examine shocks in 2D Yukawa systems to provide a deeper understanding of shocks in this system, and to provide insight into the recent experiment[1]. We focus our attention on the influence of kinetic aspects of the plasma, such as viscosity and finite mean-free-path effects. We examine two types of shocks. First, the shock wave is generated by an external electric field acting on the dust particles, giving rise to a shock wave as obtained in a laboratory experiment (with a wire). Second, we generate a shock wave by the displacement of a two-dimensional piston at constant velocity, producing a steady-state shock wave.

We find that experiment-like shock waves propagate in a highly *non-steady* state, which suggests a careful re-examination of the R-H relations in the context of non-steady shocks. And, interestingly, steady-state shock waves show an oscillatory pattern in the density, which we attribute to the dispersive effect of the dusty plasma.

A shock wave propagates (to the right) in a dusty plasma simulation. Colors show high (red) and low (blue) pressure zones.



[1] N. P. Oxtoby, E. J. Griffith, C. Durniak, J. F. Ralph and D. Samsonov. Ideal Gas Behavior of a Strongly Coupled Complex (Dusty) Plasma. *Phys. Rev. Lett.* **111**, 015002 (2013).

Dynamics of Laser-excited Argon Clusters

M. Moll[1], Th. Bornath[2], V. P. Krainov[3] and M. Schlanges*[1]
[1]Universität Greifswald, Germany
[2]Universität Rostock, Germany
[3]Moscow Institute for Physics and Technology, Russia

During the last years, there has been an impressive progress in the investigation of laser-matter interaction. In this field, a special topic is the interaction of intense laser radiation with clusters. Strongly coupled nanoplasmas at high density are created during the excitation of nanometer-sized atomic clusters with femtosecond laser pulses. The heating and expansion of these clusters as well as the ionization up to high charge states can be investigated with a modified nanoplasma model [1]. In the frame of this model, the different processes of the laser-cluster interaction are described by a coupled set of rate equations and hydrodynamic equations.
In simulations, often only ground states are considered in the rate equations describing the ionization dynamics. However, the inclusion of excited states may lead to substantially changed ionic charge states [2]. Here we present results for argon clusters from an extended nanoplasma model taking into accound both excitation and deexcitation processes. In our contribution, the influence of these processes on the ionization dynamics, on the population of excited states and on X-ray emission is discussed. Further, the dependence of various plasma parameters on the initial cluster size, the laser intensity and the pulse width are investigated and results from a double-pulse excitation scheme are presented.

*schlanges@physik.uni-greifswald.de

[1] P. Hilse, M. Moll, Th. Bornath, and M. Schlanges, *Laser-Cluster-Interaction in a Nanoplasma-Model with Inclusion of Lowered Ionization Energies*, Laser Phys. **19**, 428 (2009).

[2] S. Micheau, H. Jouin and B. Pons, *Modified nanoplasma model for laser-cluster interaction*, Phys. Rev. A **77**, 053201 (2008).

Waves in a Strongly Coupled 2D Superparamagnetic Dusty Plasma

M. Rosenberg[a], G. J. Kalman[b], P. Hartmann[b,c], Z. Donko[b,c] and S. Kyrkos[d]
[a]University of California, San Diego, La Jolla, CA 92093, U.S.A.
[b]Boston College, Chestnut Hill, MA 02467, U.S.A.
[c]Wigner Research Centre for Physics, Hungarian Academy of Sciences,
H-1525 Budapest, Hungary
[d]Lemoyne College, Syracuse, NY 13214, U.S.A.

In a two-dimensional (2D) dusty plasma composed of superparamagnetic grains and immersed in an external magnetic field the charged dust grains interact via a screened Coulomb (Yukawa) interaction and a magnetic dipole-dipole interaction. Because the magnetic dipole moment of the grains is induced by the magnetic field **B**, the dipole moments all lie along **B**. When **B** is tilted with respect to the normal to the dust layer, the interaction between the grains becomes anisotropic. At a critical angle it also changes from repulsive to attractive.

We have considered the behavior of waves in the strongly coupled liquid phase of this system [1] by analytic methods and through molecular dynamics (MD) simulations. The theoretical approach uses a reformulated Quasi-Localized Charge approximation (QLCA) that can treat dipole interactions. We confine our analysis to magnetic tilt angles such that the interaction remains repulsive in the dust layer, which allows for a stable equilibrium.

The QLCA dispersion relations show reasonably good agreement with the dispersion relations obtained from the fluctuation spectra generated by the MD simulations. The wave dispersion relations depend on the direction of propagation in the layer and the relative strengths of the magnetic dipole and Yukawa interactions. In general, the wave sound speeds increase as the relative strength of the magnetic dipole interaction increases. We discuss possible experimental parameter regimes where such effects might be observed.

We explore two new directions. One relates to the crystalline state and how different lattice structures can arise and how they affect wave behavior. The second relates to possible coupling between in-plane and out-of-plane polarized modes in a quasi-2D liquid phase, taking into account the effect of an external potential that confines the layer.

Work partially supported by NSF and NASA.

[1] P. Hartmann, Z. Donko, M. Rosenberg and G. J. Kalman, *Phys. Rev. E* **89**, 043102 (2014): DOI: 10.1103/PhysRevE.89.043102

Defining and Measuring the Coupling Strength in Coulomb and Yukawa Plasmas

T. Ott* and M. Bonitz
Institute for Theoretical Physics and Astrophysics
University of Kiel, Germany

Strongly coupled systems have become a focal point of plasma research in recent years as several experimental setups such as dusty plasmas, trapped ions, and ultracold plasmas have become available to study them. The definition of ”correlation” or ”coupling strength”, however, faces some obstacles when precise measurements of charge states and temperatures are not feasible or when the interaction between the strongly coupled species is screened, e.g., by electrons. The straightforward use of the Coulomb coupling parameter $\Gamma = Q^2/(ak_BT)$ becomes impossible under these circumstances.

In this contribution, we propose two consistent (and mutually compatible) approaches for defining and measuring the coupling strength in Coulomb and Yukawa One-Component Plasmas based on a purely structural quantity, the radial pair distribution function (RPDF). The RPDF is a relatively simple measure of the structure of a system and is often accessible in experiments by direct observation or indirectly through the static structure factor. Our approach is based on the observation that the build-up of correlation from a weakly coupled system proceeds in two steps: First, a space around each particle becomes devoid of other particles (correlation hole), and second (upon further increase of the coupling), a shell structure emerges around each particle. Using molecular dynamics simulation, we present a systematic study for the dependence of these features of the RPDF on the system state.

*ott@theo-physik.uni-kiel.de

Quantum Bound for Shear Viscosity of Strongly Coupled Electron and Dusty Plasmas

V.E.Fortov[1,2] and V.B.Mintsev[2]*
[1]Joint Institute for High Temperatures RAS,
125412, Moscow, Russia
[2]Institute of Problems of Chemical Physics RAS,
142432, Chernogolovka, Russia

String theory methods led to the hypothesis that the ratio of shear viscosity coefficient to volume density of entropy of any physical system has a lower bound [1].

$$\frac{\eta}{s} \geq \frac{\hbar}{4\pi k_B} = Q_L = 6.08 \cdot 10^{-13}\, K \cdot s$$

This work is devoted to analysis of the behavior of the shear viscosity of strongly coupled electromagnetic [2] and dusty [3] plasmas. Systems with strong coupling have a small viscosity compared to weakly coupled plasmas in which the viscosity is proportional to the mean free path.

Today a huge array of experimental data on the thermodynamic, transport and optical properties of strongly coupled plasma was received, but there are no direct measurements of viscosity [2]. For our purposes experimental data on measurements of electrical conductivity of hydrogen, deuterium and rare gases under intense shock compression and under quasiisentropic compression in multistep loading up to megabar pressures are the most interesting. The data on hydrogen, deuterium and helium-hydrogen mixture, received in the region of "metallization" at P~150 GPa in different experimental systems by the method of quasiisentropic compression reach the values η/s ~(0.3-10). Thereby, the hydrogen plasma in the region of "metallization" possesses the lowest values of the shear viscosity to the entropy ratio. Note that in this case we have an extremely high value of the coupling parameter - Γ~20-80. It is shown, that the data on electrical conductivity of strongly coupled electromagnetic plasma, confirm the tendency of decreasing of the viscosity η/s with an increase in the correlation (Γ) and thus confirm trend of the transition of the physical system to the perfect frictionless fluid with the increasing of the interparticle interaction.

Measurements of viscosity for weakly correlated dusty-plasma systems [3] are discussed. An approximation for the estimation of viscosity constants is proposed. The measured viscosity constants are compared with theoretical estimates and numerical data.

*minvb@icp.ac.ru

[1] P. Kovtun, D. T. Son and A. O. Starinets. Viscosity in Strongly Interacting Quantum Field Theories from Black Hole. Physics. *Phys. Rev Letters,* 94, 111601, 2005.

[2] V.E.Fortov and V.B.Mintsev. Quantum Bound of the Shear Viscosity of a Strongly Coupled Plasma. *Phys. Rev Letters,* 109, 055002, 2012.

[3] V.E.Fortov, O.F.Petrov, et al. Viscosity of a Strongly Coupled Dust Component in a Weakly Ionized Plasma. *Phys. Rev Letters,* 111, 125004, 2013.

Electron Oscillation Damping in Ultracold Neutral Plasmas

Wei-Ting Chen and Jacob L. Roberts
Colorado State University
Fort Collins, CO 80523, U.S.A.

Ultracold neutral plasmas are formed by photoionizing laser cooled atoms with neutral atom temperatures on the order of 10s of μK. After photoionization, a fraction of the newly-ionized electrons escape from the plasma region before the resulting positive space charge slows this escape. This results in a plasma with confined electrons and cold (~1K) ions. The initial kinetic energy of the electrons in these plasmas is determined by the wavelength of the photoionizing laser. For our system, the initial ionization energy can be set such that $\Delta E_{ionization}=k_B*(1\text{-}1000K)$. Thus, the initial kinetic energy of the electrons can be tuned over a wide range experimentally.

For the densities of the ultracold neutral plasmas in our apparatus (10^7-10^8 cm^{-3}, depending on the experimental conditions) it is possible to induce an oscillation of the electron component of the plasma as a whole[1] by applying external electric field pulses to the plasma. These pulses can be applied so that their duration is short compared to the inverse plasma frequency of the electrons. By applying pairs of these pulses with a deliberately chosen delay time between the two pulses, the oscillation frequencies and the damping rates of these oscillations can be measured. The first electric field pulse initiates the electron motion while the second can either increase or decrease the oscillation amplitude depending on the phase of the oscillation at the time of the second pulse. Since the electron oscillations result in electrons escaping from the plasma, this increase or decrease in oscillation from the second pulse can be measured experimentally.

We expect that the damping of these oscillations will be primarily due to electron-ion collisions over ranges of ultracold plasma parameters. Thus, the damping rate is expected to yield information about the electron-ion collision rate. Ultimately, we plan to measure the oscillation damping rate for parameters where the electrons will be influenced by strong coupling (Γ=0.2, or possibly somewhat higher). Before doing so, however, we measured the damping rate at higher electron temperatures (100K-250K) to test our understanding of the damping rate. The measured damping rate scaled qualitatively as expected for electron-ion collisions as a function of electron temperature and density, but the measured damping rate was over an order of magnitude faster than a standard calculation[2] would suggest. We will present the results of our experimental measurements of this electron damping rate as well as possible mechanisms for the observed damping rate being faster than expected. We will also discuss planned extensions of these measurements to ultracold neutral plasmas where strong-coupling influence in the electron component is anticipated.

*Jacob.Roberts@colostate.edu. We acknowledge support from the AFOSR.

[1] Truman M. Wilson, Wei-Ting Chen, and Jacob L. Roberts, Density-dependent response of an ultracold plasma to few-cycle radio-frequency pulses, *Phys. Rev. A* **87**, 013410 (2013).
[2] L. Spitzer, Jr.,*Physics of Fully Ionized Gases*, (Dover, New York, 1962).

Investigation of the electrons temperature in mixtures of noble gases

Y.A Ussenov*, M.K. Dosbolayev, A.U. Utegenov, T.S.Ramazanov
IETP, al-Farabi Kazakh National University, Al-Farabi 71,
Almaty 050040, Kazakhstan

Investigation of the structural and dynamical properties of the plasma-dust formations in mixtures of noble gases showed that with the addition of a small amount of gas impurity, the properties of dust structures greatly changed [1-3]. During the experiments in CCRF discharge it was found that a small admixture of argon to helium leads to crystallization of the plasma structure. That is contrast to experiment with pure helium. The explanation of this behavior of plasma-dust structures in the background plasma of the gas mixture requires knowledge of the main discharge characteristics such as the electron temperature under different experimental conditions and its changes with the addition of heavy argon to the helium gas.

In this paper the results of a study of the electron temperature of the buffer plasma in mixtures of noble gases (helium + argon) in capacitively coupled radiofrequency (CCRF) discharge are presented. Measurements using an RF compensated electric probe [4-5] in the pressures in the range of 0.1-0.6 Torr were performed. Comparison of the results shows that addition a small amount of argon to the helium leads to an increase in the electron temperature.

*yerbolat@physics.kz

[1] T.S. Ramazanov, S.A. Maiorov, K.N. Dzhumagulova, M.K. Dosbolayev, A.N. Jumabekov, *Physics of Plasmas* **3** (2008) 120-127.

[2] T.S.Ramazanov, T.T. Daniyarov, S.A. Maiorov, S.K. Kodanova, M.K. Dosbolayev and E.B. Zhankarashev, *Contrib. Plasma Phys*. 51 (2011) 505-508.

[3] M.K. Dosbolayev, A.U. Utegenov, T.S. Ramazanov, T.T. Daniyarov , *Contrib. Plasma Phys*., 53 (2013) 426-431.

[4] F. F. Chen: *Physics of Plasmas*, 8 (2001) 3029.

[5] F. F. Chen : *Plasma Sources Sci. Technol*. 18 (2009) 035012.

Localized viscous heating observed in a two-dimensional strongly coupled dusty plasma

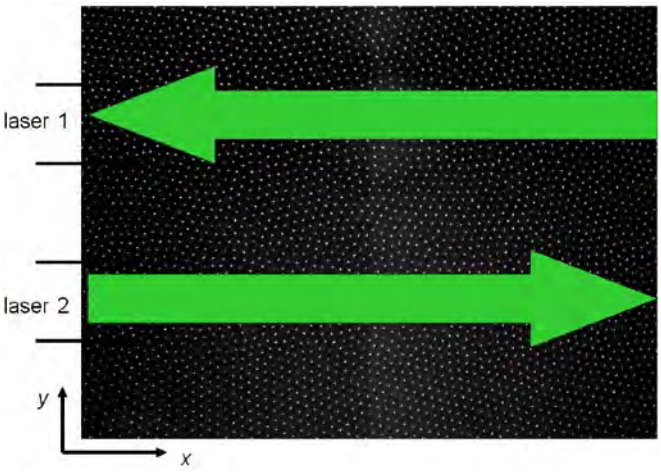
Yan Feng,* John Goree and Bin Liu
Department of Physics and Astronomy, The University of Iowa
Iowa City, IA 52242, U.S.A.

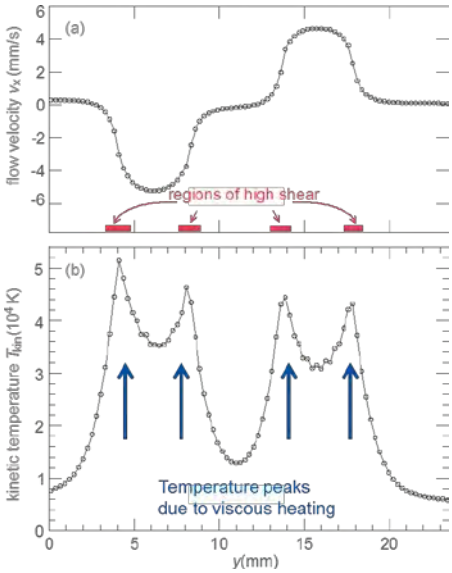
Viscous heating is conversion of directed energy to thermal energy in a liquid when there is a shear in the velocity profile. It occurs locally at a rate proportional the square of the velocity shear. For this reason, one might expect to observe a hot spot in a region of high shear. However, such a hot spot is never seen in an ordinary liquid such as water because thermal conduction carries the generated heat away too rapidly for the temperature profile to change detectably.

We have found that we can observe such a hot spot in a liquid-like strongly coupled plasma. To do this, we used a dusty plasma, which is a mixture of highly charged polymer microspheres, electrons, ions, and neutral gas. The microspheres were electrically levitated as a single horizontal layer. They were imaged by video microscopy.

We drove two counter-propagating flows with a pair of laser beams that were displaced so that the flow had a shear region between them. Using image analysis methods, we measured individual particle velocities. We then calculated the local flow velocity as the first moment of the particle velocities, and the local kinetic temperature as the second moment.

The resulting profiles have profound peaks, which we interpret as the signature of localized viscous heating. A calculation of the dimensionless Brinkman, Prandtl and Eckert numbers confirms this interpretation.





Work supported by NSF and NASA.
*Current address: LANL

[1] Feng Goree and Liu, PRL 109, 185002 (2012).

Thursday Posters

SCCS 2014
Abstracts

Friday, August 1st

Quasi-magnetization of rotating dusty plasmas

P. Hartmann[1]*, Z. Donkó[1], T. Ott[2], H. Kählert[2], M. Bonitz[2]

[1] Wigner Research Centre for Physics, Hungarian Academy of Sciences, Budapest, Hungary

[2] Christian-Albrechts-Universität zu Kiel, Germany

We have constructed a new experimental setup to realize and observe rotating dusty plasmas in a co-rotating frame. The "RotoDust" setup is able to create effective magnetizations, mimicked by the Coriolis inertial force, in a strongly coupled dusty plasma that are impossible to approach with superconducting magnets. At the highest rotation speed, we have achieved effective magnetic fields of 3200 T [1]. The effective magnetization $\beta = \omega_c/\omega_p$ (ratio of cyclotron to plasma frequency) reaches 0.76 which is typical for many strongly magnetized and strongly correlated plasmas in compact astrophysical objects [2].

The analysis of the wave spectra as observed in the rotating frame clearly shows the equivalence of the rotating dust cloud and a magnetized plasma. The $k \rightarrow 0$ gap frequency is found at twice the rotation frequency, which corresponds to the cyclotron frequency in a magnetized system. The excellent agreement with wave spectra from molecular dynamics simulations supports the applicability of this experimental technique to emulate large magnetic effects. Moreover, the simulations confirm that the setup can be used for quantitative studies of extended, macroscopic strongly coupled magnetized plasmas. While we have focused on the fundamental current fluctuation spectra, several other plasma properties, including diffusion [3] or viscosity, are affected by a strong magnetic field, and are now accessible experimentally. The RotoDust setup opens the way for these investigations in the near future.

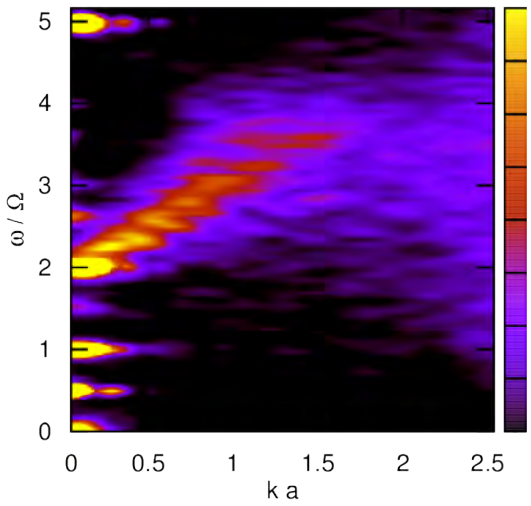


Figure 1: *Longitudinal current fluctuation spectra at angular velocity* $\Omega = 23.3$ *rad/s.*

*hartmann.peter@wigner.mta.hu

[1] P. Hartmann, Z. Donkó, T. Ott, H. Kählert, M. Bonitz *Magnetoplasmons in rotating dusty plasmas* Phys. Rev. Lett. **111**, 155002 (2013)

[2] H. Kählert, J. Carstensen, M. Bonitz, H. Löwen, F. Greiner, and A. Piel *Magnetizing a complex plasma without a magnetic field* Phys. Rev. Lett. **109**, 155003 (2012)

[3] T. Ott and M. Bonitz *Diffusion in a strongly coupled magnetized plasma* Phys. Rev. Lett. **107**, 135003 (2011)

Experimental Studies of Two-dimensional Melting in Dusty Plasma

O.F. Petrov[1,2], V.E. Fortov[1,2], M.M. Vasiliev[1], Y. Tun[2], K.B. Stacenko[1], O.S. Vaulina[1,2], E.V. Vasilieva[1], E.M. Lisin[1] and M.I. Myasnikov[1]
[1]Joint Institute for High Temperatures RAS, Moscow, Russia
[2]Moscow Institute of Physics and Technology, Dolgoprudny, Russia
ofpetrov@ihed.ras.ru

The charged dust system represent a non-neutral or quasi-neutral systems (dusty plasmas) containing micron-sized particles of a substance with electrical charges up to 10^2-10^5e. As a result of strong interaction, the dust particles may form the ordered structures of liquid and crystal types. The laboratory dusty plasma is the unique object for studying the structures, phase transitions and transport phenomena on the "kinetic level".
The phase transitions in quasi-two-dimensional dust structures suspended in rf discharge were studied. Two-stage melting is observed experimentally in a confined monolayer of dust particles in plasma. The experimental results have revealed the existence of hexatic phase as well as solid-to-hexatic phase and hexatic-to-liquid transitions. The pair correlation and bond-angular correlation functions, the number of topological defects, the pair potentials and the excess entropy are measured and analyzed. The bond-orientational correlation functions show a clear solid-to-hexatic-to-fluid transition, in perfect agreement with the Kosterlitz-Thouless-Halperin-Nelson-Young theory, and the ensemble's entropy demonstrates sharp change around transition. The spatial distribution of pair interparticle interaction forces was recovered by the original method based on solving the inverse problem using Langevin equations. The measured phase-state points with the theoretical phase diagram of two-dimensional Yukawa system have been obtained.

This work was partially supported by the Russian Foundation for Basic Research (Projects No. 13-02-01393 and 13-02-12256) and by the Program of the Presidium of RAS "Matter under High Energy Densities".

First Principles Nonequilibrium Plasma Mixing

C. Ticknor

Theoretical Division, Los Alamos National Laboratory
Los Alamos, New Mexico 87545, USA

We have performed nonequilibrium classical and quantum-mechanical molecular dynamics simulations that follow the interpenetration of deuterium-tritium (DT) and carbon (C) components through an interface initially in hydrostatic and thermal equilibrium. We concentrate on the warm, dense matter regime. The classical treatment employs a Yukawa pair-potential with the parameters adjusted to the plasma conditions, and the quantum treatment rests on an orbital-free density functional theory at the Thomas-Fermi-Dirac level. For times greater than about a picosecond, the component concentrations evolve in accordance with Fick's law for a classically diffusing fluid with the motion, though, described by the mutual diffusion coefficient of the mixed system rather than the self-diffusion of the individual components. For shorter times, microscopic processes control the clearly non-Fickian dynamics and require a detailed representation of the electron probability density in space and time.

Is the compressibility positive or negative in a strongly-coupled dusty plasma?

John Goree and W. D. Suranga Ruhunusiri
Department of Physics and Astronomy, The University of Iowa
Iowa City, IA 52242, U.S.A.

Theory and experiments disagree regarding the sign of the compressibility β for a strongly-coupled component in a multicomponent plasma. This discrepancy is found in the dusty plasma literature, where experiments allow direct comparison to theory. The dust particles are strongly coupled with a large Γ, while the electrons and ions that share the same volume are weakly coupled. Compression of the dust component occurs in a dust acoustic wave (DAW), and it is easily measured by video microscopy.

The compressibility of a substance of number density n, pressure P, and volume V is:

$$\beta \equiv -(1/V)\partial V / \partial P = (1/n)\partial n / \partial P$$

In most substances, compressibility must be positive. Otherwise there would be an explosive instability. In a multicomponent plasma, however, one could entertain the idea that the compressibility of a single component could be negative, provided that the restoring force from charge separation overwhelms the destabilizing effect.

Three theories of the DAW, for conditions with strong coupling of the dust, all assume that β is *negative*. [1-3] These theories use a multi-fluid model to compute the wave dispersion relation with a self-consistent macroscopic electric field for the wave. For the dust component, they use a compressibility found from an OCP or Yukawa-OCP approach.

Three experimental papers, on the other hand, have achieved a satisfactory agreement of their DAW experimental data with a theoretical dispersion relation that assumes β is *positive* [4-6]. In some cases, these authors assumed an ideal-gas law for the dust, but with an ad-hoc increase in the dust temperature in order to reduce β to achieve an agreement with experiment.

This remarkable discrepancy in the literature has apparently gone unnoticed until now. To help resolve the discrepancy, we performed an experiment aimed at precisely determining β for the dust, including its sign. In doing so, we take into account the uncertainty ranges of all experimentally measured parameters. We rely on a theoretical dispersion relation that includes as many experimentally relevant processes as practical. The result will be presented at this conference.

Work supported by NSF and NASA.

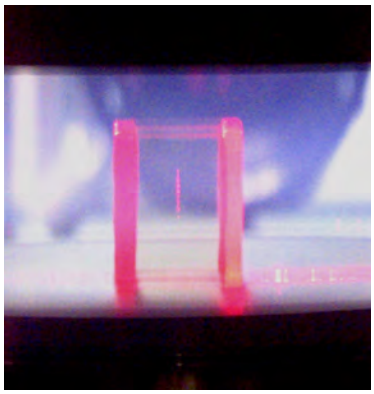
[1] M. Rosenberg and G. Kalman, *Physical Review E*, 56:7166, 1997.
[2] M. S. Murillo, *Physics of Plasmas*, 5:3116, 1998.
[3] P. K. Kaw and A. Sen, *Physics of Plasmas*, 5:3552, 1998.
[4] J. D. Williams, E. Thomas Jr., and L. Marcus, *Physics of Plasmas*, 15:043704, 2008.
[5] V. V. Yaroshenko, V. Nosenko, and G. E. Morfill, *Physics of Plasmas*, 17:103709, 2010.
[6] T. M. Flanagan and J. Goree, *Physics of Plasmas*, 17:123702, 2010.

Chains (Strings) in Complex Plasma

Truell W. Hyde, Jay Kong, and Lorin Matthews
Center for Astrophysics, Space Physics & Engineering Research (CASPER)
Baylor University, Waco, TX 76712, U.S.A.

Examination of collective phenomena within complex plasma allows investigation into the fundamental physics behind the strong correlation effects observed across a broad range of systems. Recently, research into the micro-excitations of dust in vertical chain bundles has increased due to interest in other 2+1 D liquids sharing similar characteristics. This is particularly true for systems providing external field alignment of the bundle. Most such chain motion is created due to (a) strong vertical interparticle coupling creating particle alignment within the chain, (b) topological constraints arising from the structure of the confinement, (c) local strain-induced stresses which can induce particle hopping and overall chain motion and/or (d) interchain forces. This paper will discuss the manner in which vertical and horizontal coupling tends to align vertical chain(s) and the topological constraints arising from anisotropic confinement. Specifically, single and multiple vertically aligned dust particle chains produced employing a glass box placed on the lower electrode of a GEC rf reference cell will be examined. It will be shown that transitions from a single 1D vertical chain to a 2-fold zigzag structure and 3-, 4-, and 5-fold helical structures can occur. Both theoretical and experimental results will be used to better define the role that system confinement plays in the physics underlying the overall macroscopic behavior.

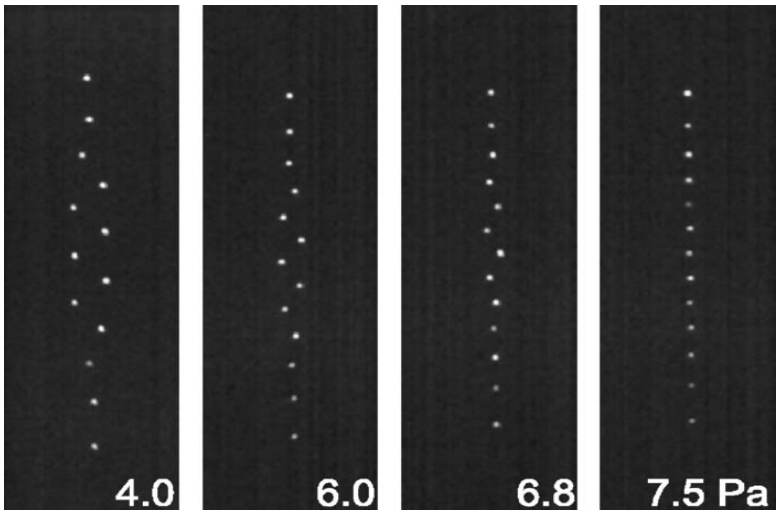
*Truell_Hyde@baylor.edu



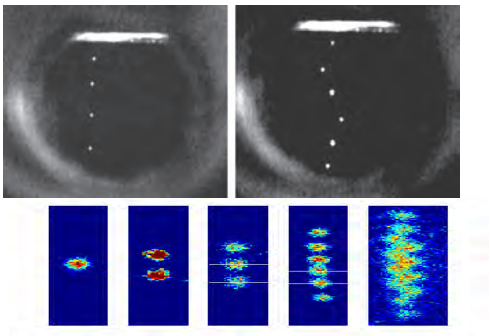
[1] Ke Qiao, Jay Kong, Eric Van Oeveren, Lorin S. Matthews and Truell W. Hyde *Mode Couplings and Resonance Instabilities in Dust Clusters*, Physical Review E, 88, 043103, 2013.

[2] Truell W. Hyde, Jay Kong and Lorin Matthews, *Helical Structures in Vertically Aligned Dust Particle Chains in a Complex Plasma,* Physical Review E, 87, 053106, 2013.

[3] Jay Kong, Ke Qiao, Jorge Carmona-Reyes, Angela Douglass, Zhuanhao Zhang, Lorin Matthews and Truell W. Hyde, *Vertical Interaction Between Dust Particles Confined within a Glass Box in a Complex Plasma*, IEEE Transactions on Plasma Science, 41, 4, 2013.



[4] W.Guo, D.Jin and HJ.Maris, *A Study of the Motion of Single Electrons in Liquid Helium*, Phonons 2007, Journal of Physics: Conference Series 92, 012001, 2007.



Signe Seidelin and John Chiaverini/NIST

Electrostatics in low-dielectric constant colloidal systems : ultra-long range, electroneutrality violation and self-induced anisotropy

C. P. Royall
University of Bristol
HH Wills Physics Laboratory, Tyndall Avenue, Bristol, BS8 1TL, UK.
School of Chemistry, Cantock's Close, Bristol, BS8 1TS, UK.
Centre for Nanoscience and Quantum Information, Tyndall Avenue, Bristol, BS8 1FD, UK.

Colloidal particles are typically suspended in water. Given typical ionic radii of a few Angstroms, water's dielectric constant leads to ionic binding energies of a few times the thermal energy k_BT. In such systems, most ions dissociate, leading to molar ionic strengths. Here we consider systems in which the solvent dielectric constant is around 2-5 [1]. This leads to strong ion binding energies of tens of k_BT which in turn results in weak charging and ultra-low ionic strengths (10^{-9} – 10^{-4} M) [1]. We review some unusual behaviour of these strong Coulomb coupling colloidal systems. Under some conditions, these systems are remarkably well described by Yukawa interactions [2]. The strong ion-colloid coupling can lead to unusual phenomena such as re-entrant melting [3]. Meanwhile at ultra-low ionic strengths anomalous "low-density crystals" are formed under conditions which Yukawa theory fails to predict such structures [2]. The origin of these low-density crystals remains elusive, although a breakdown in charge neutrality may provide an explanation. Attractions between the colloidal particles can be induced by adding polymer. Such attractions one expects will compete with repulsive electrostatic interactions [4]. However a complex coupling of ions and binding sites leads to an anisotropic charge distribution on the colloids. Remarkably, here the ionic diffusion time is comparable to relaxation time of micron-sized colloids [5].
*paddy.royall@bristol.ac.uk

[1] A. Ivlev, H. Löwen, G. E. Morfill, and C. P. Royall, *Complex Plasmas and Colloidal Dispersions: Particle-resolved Studies of Classical Liquids and Solids* World Scientific Publishing Co., Singapore Scientific (2012).
[2] C. P. Royall, M. E. Leunissen, and A. van Blaaderen, *A new colloidal model system to study long-range interactions quantitatively in real space* J. Phys.: Condens. Matter, **15** S3581-S3596, (2003).

[3] C. P. Royall, M. E. Leunissen, A.-P. Hyninnen, M. Dijkstra, and A. van Blaaderen, *Re-entrant melting and freezing in a model system of charged colloids* J. Chem. Phys. **124** 244706, (2006).

[4] C. P. Royall, D. Aarts, and H. Tanaka, *Fluid structure in colloid-polymer mixtures: the competition between electrostatics and depletion.* J. Phys.: Condens. Matter, **17** S3401-S3408 (2005).

[5] C. L. Klix, K. Murata, H. Tanaka, S. Williams, A. Malins, and C. P. Royall, *Novel kinetic trapping in charged colloidal clusters due to self-induced surface charge organization* Scientific Reports, **3** 2072, (2013).

Experimental determination of the sound speed and Grüneisen coefficient of shock-compressed liquid deuterium‡

P.M. Celliers,[1*] D.E. Fratanduono,[1] D.H. Munro,[1] T.R. Boehly,[2] D.G. Hicks,[3] J.H. Eggert,[1] and G.W. Collins[1]

[1]Lawrence Livermore National Laboratory
Livermore, CA 94551, U.S.A.
[2]University of Rochester – Laboratory for Laser Energetics,
Rochester, NY 14623, U.S.A.
[3]University of Melbourne, Melbourne, Australia

In the last decade many Hugoniot experiments on hydrogen isotopes have produced a large data set, both along the cryogenic principal Hugoniot[1,2] and along precompressed Hugoniots[3]. A recent accurate calibration of the shock wave equation of state of alpha-quartz[4] can be combined with a new data analysis technique to enable the experimental determination of both the sound speed and Grüneisen coefficient along the Hugoniot for appropriately designed laser-driven shock Hugoniot experiments. It turns out that an impedance-match Hugoniot data set for deuterium along the cryogenic principal Hugoniot[2], collected more than 10 years ago, is amenable to this new analysis. By revisiting this decade-old data set we have extracted both the sound speed and Grüneisen coefficient of shock compressed deuterium along the cryogenic principal Hugoniot from 50 to 200 GPa.

‡This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.
*celliers1@llnl.gov

[1] M. D. Knudson, D. L. Hanson, J. E. Bailey, C. A. Hall, J. R. Asay, and C. Deeney, Phys Rev. B **69**, 144209 (2004).
[2] D. G. Hicks, T. R. Boehly, P. M. Celliers, J. H. Eggert, S. J. Moon, D. D. Meyerhofer and G. W. Collins, Phys. Rev. B **79**, 014112 (2009).
[3] P. Loubeyre, S. Brygoo, J. Eggert, P. M. Celliers, D. K. Spaulding, J. R. Rygg, T. R. Boehly, G. W. Collins, and R. Jeanloz, Phys. Rev. B **86**, 144115 (2012).
[4] M. D. Knudson and M. P. Desjarlais, Phys. Rev. B **88,** 184107 (2013).

Pulsed power methods to access off-Hugoniot states in liquids

M.D. Knudson,[1]* M.P. Desjarlais,[1] R.W. Lemke,[1] K. Cochrane,[1] A. Becker,[2] and R. Redmer[2]
[1]Sandia National Laboratories
Albuquerque, NM 87123, U.S.A.
[2]Institut für Physik, Universität Rostock
Rostock, Germany

Recently we have been exploring various pulsed power experimental concepts to access off-Hugoniot states in liquids at the Sandia Z Accelerator. One very promising technique utilizes a so-called shock-ramp platform. Here a relatively small gap is introduced between the ramp compression load electrode and a liquid sample cell. The accelerator is configured to deliver a two-step current pulse; the first step accelerates the electrode to a reasonably constant velocity, which upon impact with the sample cell creates a well-defined shock, while the subsequent current rise produces ramp compression from the initially shocked state. This technique may make it possible to achieve relatively cool (~1000 K), high compression states (~10 fold compression). This would allow experimental access to the region of phase space where hydrogen is predicted to undergo a first-order liquid-liquid phase transition from an insulating molecular-like liquid to a conducting atomic-like fluid; the so-called plasma phase transition (PPT). In this talk we will discuss the development of the liquid shock-ramp platform, survey the various theoretical predictions for the liquid-liquid transition in hydrogen, and present the results of any experiments performed that access this region of phase space.

*mdknuds@sandia.gov

Thermal conductivity measurements of CH and Be by refraction-enhanced x-ray radiography

Y. Ping[1], J. King[2], O. L. Landen[1], R. Freeman[2], T. Boehly[3], G. W. Collins[1]
[1]Lawrence Livermore National Laboratory, Livermore, CA, USA
[2]College of Mathematical and Physical Sciences, Ohio State University, Columbus, Ohio, USA
[3]LLE, U. Rochester, Rochester, NY, USA

Transport properties of warm dense matter are important for modeling the growth of hydrodynamic instabilities near the fuel-ablator interface in an ICF capsule, which determines the mix level in the fuel and thus is critical for successful ignition. A novel technique, time-resolved refraction-enhanced x-ray radiography, has been developed to study thermal conductivity at an interface [1]. Experiments using OMEGA laser have been carried out for CH/Be targets isochorically heated by x-rays to measure the evolution of the density gradient at the interface due to thermal conduction. The sensitivity of this radiographic technique to discontinuities enabled observation of shock/rarefraction waves propagating away from the interface. The radiographs provide enough constraints on the temperatures, densities and scale lengths in CH and Be, respectively. Preliminary data analysis suggests that the thermal conductivities of CH and Be at near solid density and a few eV temperature are higher than predictions by the commonly used Lee-More model. Detailed analysis and comparison with various models will be presented.

The work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Security, LLC, Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

*ping2@llnl.gov

[1] Y. Ping, O. L. Landen, D. G. Hicks, J. A. Koch, R. Wallace, C. Sorce, B. A. Hammel, G. W. Collins, J. Instru. 6, P09004 (2011).

The Role of High Performance Computing in Coulomb Systems

James N. Glosli[1], David F. Richards[1], Liam G. Stanton[1], Michael P. Surh[1] and Michael S. Murillo[2],

[1]Lawrence Livermore National Laboratory, Livermore, CA 94551, USA
[2]Los Alamos National Laboratory, Los Alamos, NM 87545, USA

Molecular dynamics (MD) methods have historically played a central role in elucidating the properties of strongly coupled Coulomb Systems. MD is a non-perturbative, many-body approach that can be used to explore both equilibrium and temporal properties of many-body systems. In contrast to Monte Carlo methods, MD provides accurate dynamical information for properties such as fluctuations, collective response and transport, which can be difficult to probe experimentally. With new advancements in algorithms and increasing computational horsepower, broader classes of problems can be tackled. Recent years have shown a trend toward exploring the rich dynamics of non-equilibrium and heterogeneous systems.

In this talk, we will examine the state-of-the-art in MD algorithms and their connection to modern high performance computer platforms. We have developed a heterogeneous decomposition method for large systems, such as Sequoia-call computers, which allows for billions of particles evolved for millions of times steps.

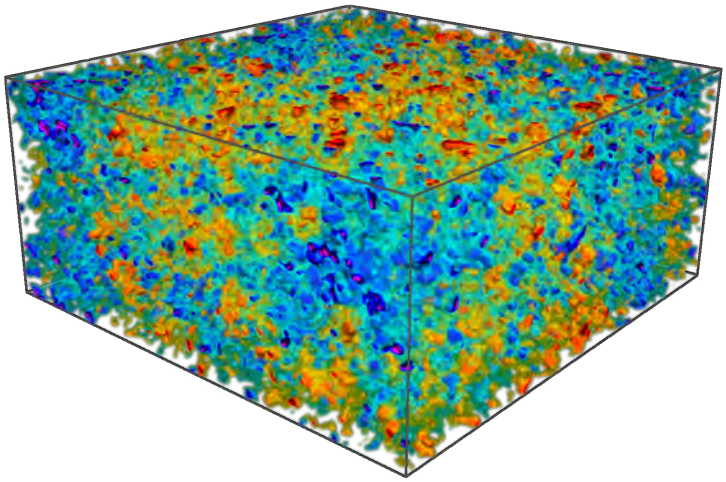


Figure: Visualization of an early ASC Dawn-sized simulation. Electron potential in a 140-million-particle simulation of a 5 keV plasma composed of deuterium/tritium and 3.5-million-electron-volt alpha particles, being heated by an argon beam.

notes

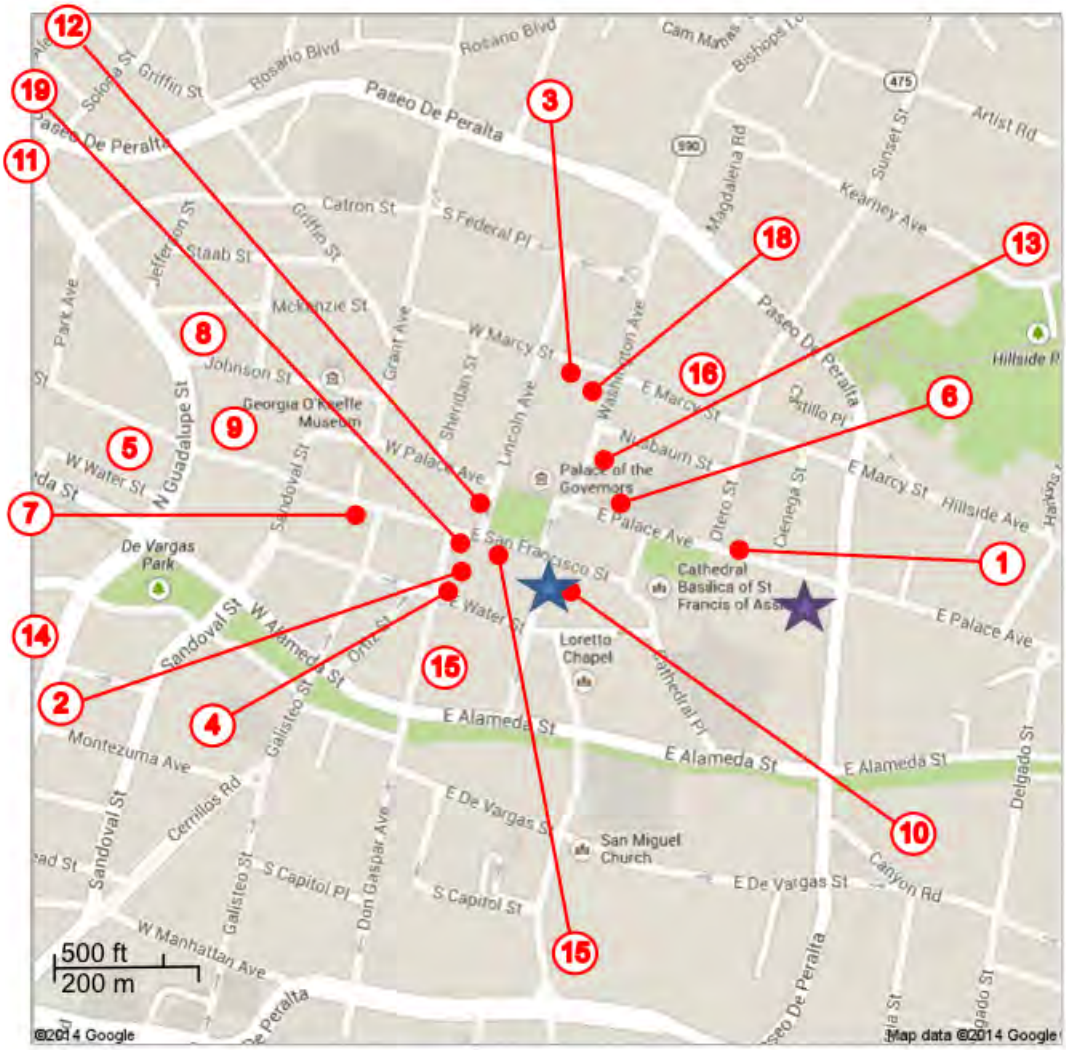
notes

notes

notes

notes

Area Map with Points of Interest

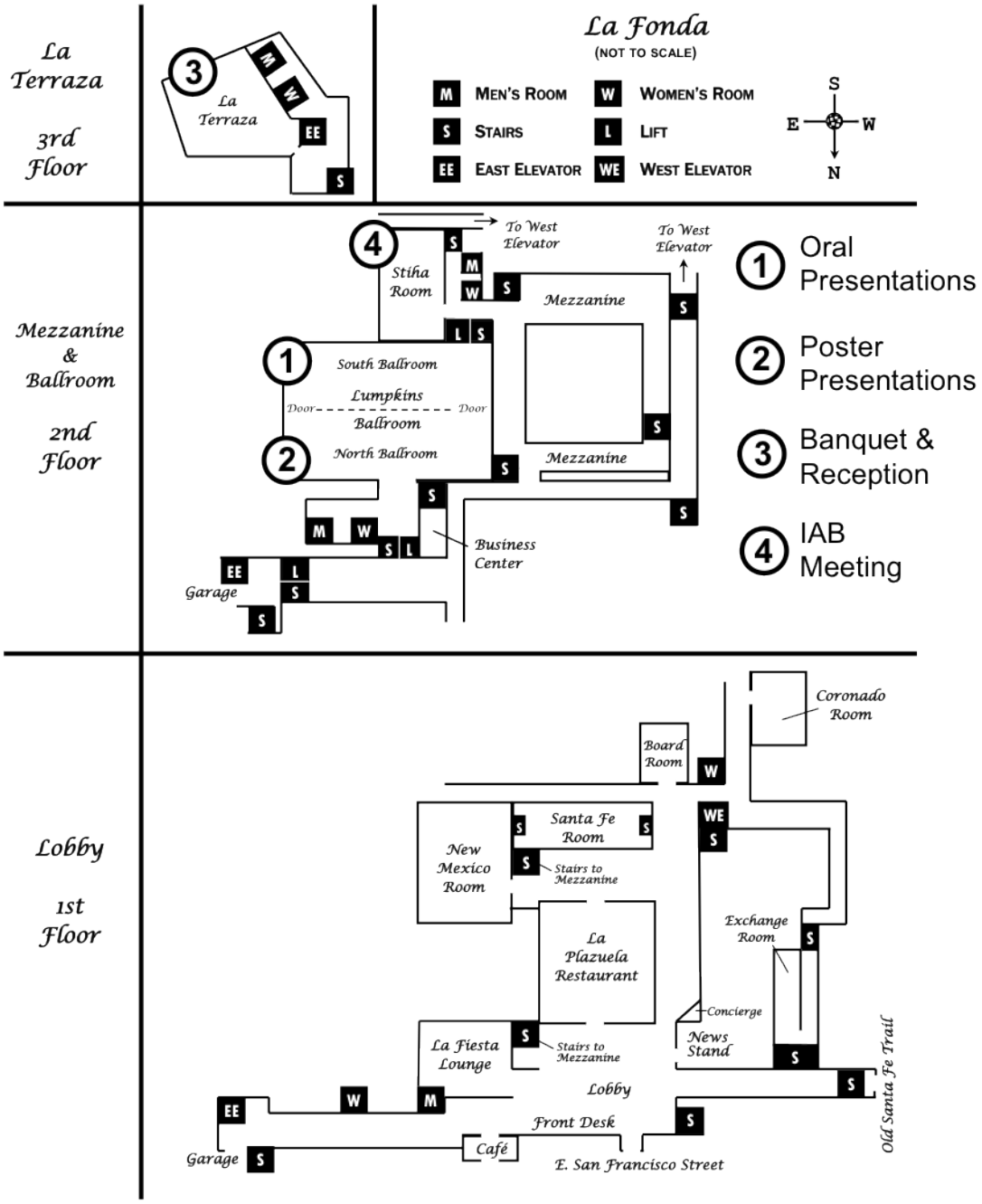


La Fonda on the Plaza **Drury Plaza Hotel**

Restaurants:

1) Palacio Cafe ($) – *Sandwiches, Breakfast*
2) Elevation Bistro ($$) – *American*
3) La Boca ($$$) – *Tapas, Spanish*
4) Cafe Pasqual's ($$) – *New Mexican*
5) Casa Chimayo Restaurant ($$) – *New Mexican*
6) The Shed ($$) – *New Mexican*
7) Tia Sophias ($) – *New Mexican (Lunch)*
8) Shohko-Cafe ($$$) – *Japanese*
9) Il Vicino ($$) – Pizza, *Italian*
10) La Plazuela at La Fonda ($$) – *New Mexican*
11) Clafoutis French Bakery ($$) – *French (Lunch)*
12) The Plaza Cafe ($$) – *New Mexican (Brunch)*
13) The Burrito Company ($) – *Mexican (Lunch)*
14) Whole Hog Cafe ($$) – *Barbeque*
15) India Palace ($$) – *Indian*
16) Sushi Land East ($$) – *Sushi*
17) Izmi Sushi Bar ($$) – *Sushi*
18) The Bull Ring ($$$) – *Steakhouse*
19) San Francisco St. Bar & Grill ($$) – *American*

Map of La Fonda on the Plaza



	Sunday	Monday	Tuesday	Wednesday	Thursday	Friday	
		Registration/Help Desk -- La Fonda's Mezzanine Level -- Opens 07:30 each day					
08:30-08:45		Welcome	Keynote Ospelkaus (Hannover)	Keynote Dharma-wardana (NRC)	Keynote Döppner (LLNL)	Invited Hartmann (SZFKI Budapest)	08:30-08:45
08:45-09:00		Keynote Collins (LLNL)					08:45-09:00
09:00-09:15						Petrov	09:00-09:15
09:15-09:30			Invited Bedell (Boston College)	Invited Schliemann (Univ. Regensburg)	Invited Gregori (Oxford)	Ticknor	09:15-09:30
09:30-09:45		Invited Nettelmann (UCSC)				Goree	09:30-09:45
09:45-10:00			Harbour	Bonitz	Clerouin	Hyde	09:45-10:00
10:00-10:15		Desjarlais	Hansen	Dubin	Plagemann	Invited Royall (Bristol)	10:00-10:15
10:15-10:30		Coffee	Coffee	Coffee	Zhilyaev/Stegailov		10:15-10:30
10:30-10:45					Coffee	Coffee	10:30-10:45
10:45-11:00		Johnson	Invited Quader (Kent State)	Dufty			10:45-11:00
11:00-11.15		Becker		Reichhardt	Invited Boronat (Barcelona)	Celliers	11:00-11.15
11:15-11:30		Bethkenhagen	Cebulla	Palo/Senatore		Knudson	11:15-11:30
11:30-11:45		Grabowski	Norman	Schoof	Bystryi	Ping	11:30-11:45
11:45-12:00		Zeng	Meyer	Dharuman	Lyon	Invited Glosli (LLNL)	11:45-12:00
12:00-12:15		Invited Yuan (NUDT)	Hamel	Zelener	Tributes to Dewitt, Rogers, Jancovici		12:00-12:15
12:15-12:30			Rudd	Silvestri		Closing Remarks	12:15-12:30
12:30-12:45		LUNCH & Informal Discussions	LUNCH & Informal Discussions IAB Luncheon (Stiha Room)	Free Time (45 minutes)	LUNCH & Informal Discussions		12:30-12:45
12:45-13:00							12:45-13:00
13:00-13:15							13:00-13:15
13:15-13:30				Board Buses			13:15-13:30
13:30-13:45				Travel to Bandelier			13:30-13:45
13:45-14:00							13:45-14:00
14:00-14:15					Invited Kählert (CAU Kiel)		14:00-14:15
14:15-14:30							14:15-14:30
14:30-14:45		Keynote Daligault (LANL)	Invited Benedict (LLNL)	Bandelier Tour	Museum Hill and Canyon Road Tour	Das	14:30-14:45
14:45-15:00						Ludwig	14:45-15:00
15:00-15:15			Mabey			Allahyarov	15:00-15:15
15:15-15:30		Belof	Markmann			Yang	15:15-15:30
15:30-15:45	Registration/Help Mezzanine Level	Starrett	Chakraborty/Trickey			Davletov	15:30-15:45
15:45-16:00		Filinov/Bonitz	Arkhipov			Ramazanov	15:45-16:00
16:00-16:15		Baczewski	Bussmann			Break	16:00-16:15
16:15-16:30		Break	Break			Poster Introductions	16:15-16:30
16:30-16:45		Poster Introductions	Poster Introductions	Travel Bandelier to Chimayo	Board Bus	Poster Session 3 Presentations (20 posters)	16:30-16:45
16:45-17:00					Travel La Fonda to Chimayo		16:45-17:00
17:00-17:15		Poster Session 1 Presentations (19 posters)	Poster Session 2 Presentations (18 posters)				17:00-17:15
17:15-17:30							17:15-17:30
17:30-17:45	Welcome			Tour El Santuario de Chimayo			17:30-17:45
17:45-18:00							17:45-18:00
18:00-18:15					Free Time		18:00-18:15
18:15-18:30	Reception La Terraza Room						18:15-18:30
18:30-18:45				Dinner at Rancho de Chimayo	Banquet La Terraza Room (18:30-22:00) Dinner served at 19:00 Poster and Student Awards		18:30-18:45
18:45-19:00							18:45-19:00
19:00-19:15						**6 Topics**	
19:15-19:30							
19:30-19:45	1. Dense and astrophysical plasmas	(includes solar, giant planets, white dwarfs, neutron stars, hydrogen, helium, equation of state, plasma phase transition, transport and optical properties)				**5 Keynote Talks (45 mins)**	
19:45-20:00							
20:00-20:15	2. Plasmas in condensed matter	(includes electron liquids in solids, plasmas in semiconductors, liquid metals, Bose condensation in Coulomb systems, ionic lattices)				**12 Invited talks (30 mins)**	
20:15-20:30							
20:30-20:45	3. Confined and mesoscopic Coulomb systems	(includes quantum dots, charged particle bilayers, dipole systems,biological systems, clusters). See also Topic 2		Board Buses		**49 Contributed talks 15 mins) ~8 in each Topic**	
20:45-20:00				Travel to Santa Fe (Arrive 21:30)			
21:00-21:15	4.High energy-density plasma in the laboratory	(includes matter at high energy-densities, laser-plasma interaction, relativistic plasmas, many-particle QED). See also Topic 1				**1 minute poster introductions in a 30 minute session 19+18+20 posters in 3 sessions**	
21:15-21:30							
21:30-21:45	5.Classical charged systems	(includes complex plasmas and colloids, electrolytes, dusty plasmas)		6. Development in theoretical methods and numerical techniques		(includes advances in theoretical methods and numerical techniques with generic applications in SCCS)	
21:45-22:00							