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During the grant period research has focused on the nonequilibrium dynamics of electrons in the presence of ions, both via basic quantum theory and via semi-classical molecular dynamics (MD) simulation. In addition, fundamental notions of dissipative dynamics have been explored for models of grains and dust, and for scalar fields (temperature) in turbulent edge plasmas. The MD simulation work was part of a long standing and continued collaboration with A. Callisti and B. Talin, University of Provence. A new collaboration with Michael Bonitz, University of Kiel, on quantum kinetic theory for metallic clusters was begun during this latest period. Multiple pairwise extended visits to the institutions occurred to optimize all resources available since the original amount requested was decreased significantly in the final award.

Quantum Kinetic Theory for Metallic Clusters

The wealth of experimental data on a wide range of metallic clusters has produced a number of theoretical challenges for a basic understanding of such systems. Two categories of such questions are those that involve dynamics of the ions as well as electrons, and those dominated by valence electron dynamics in the presence of "frozen" ions. For the first case see the section on quantum embedding below. In the second case the frozen ion configuration behaves as an inhomogeneous external confining potential for the electrons. The simplest mean field description is the nonlinear time dependent Hartree – Fock (TDHF) equation. Its classical limit would be the nonlinear Vlasov equation, but this limit does not exist due to the singular electron – ion attraction. Two routes for analysis have been explored, a direct quantum analysis of the TDHF and a semi-classical analysis of the Vlasov equation using "regularized" electron – ion Coulomb interactions. In the first case, the context of interest was metallic clusters where the confining potential of tightly bound electrons and ions was described by a simple Thomas – Fermi – Density Functional form. The TDHF was generalized formally to include a strong external pulsed laser field and the role of dynamical screening of an inhomogeneous electron cloud was discussed. The quantum kinetic equation was constructed in a gauge invariant form to accommodate a range of practical approximations for the external laser field.

Semi-classical MD Simulation

The second approach to describing the dynamics of confined or inhomogeneous electron systems is via classical mechanics with Coulomb potentials modified to represent quantum effects at short distances. The TDHF equation becomes the Vlasov equation and the corresponding stationary equation is the weak coupling hypernetted chain (HNC) integral equation. The inhomogeneous electron structure has been studied by numerical solution to the HNC equation, while the dynamics has been analyzed via time correlation functions for the electron forces on the ions. Both have been reinforced by extensive MD simulation for this regularized potential. Peculiarities such as enhanced tails of the force distributions and dynamical anti-correlation in the dynamics have been captured quantitatively by the analytic studies. However, a surprising failure of the Vlasov model (including HNC) was found at weak electron coupling, but high Z ions. The origin is traced to the tail of the force distribution and further study comprises part of the proposed research here.

The form of the regularized Coulomb potentials was studied as well, in an attempt to extend their applicability to the colder valence electrons of some metallic clusters. One approach is purely phenomenological, involving modification of the parameters in the weak coupling Kelbg form (this potential is virtually exact due to a fit to the exact solution of the two-particle problem with path integral Monte Carlo simulation; the resulting semi classical MD simulations work well even in the strong coupling regime, and fail only at temperatures below the molecule dissociation energy and for frequencies larger than the plasma frequency). We have also explored the non-perturbative approach of Feynman and Kleinert. The limitations of that variational approach have now been quantified for the plasmas of interest. More recently, regularized potentials to describe the quantum effects of confinement have been described and are the topic for continued research under the joint NSF/DOE program.

Effects of Dissipative Dynamics

The qualitative effects of two types of dissipation on dynamics have been explored: turbulence in "edge" plasmas, and inelastic collisions among mesoscopic grains. In the first case we have studied the statistical properties of the ion temperature in a turbulent plasma, using a model of stochastic advection. Standard field theoretical methods developed for turbulence in neutral fluids have been applied to the Braginskii hydrodynamics for a complex plasma of electrons and ions. Predictions for overpopulated tails in the distribution of the temperature have been made, and the possibility for their observation via spectroscopy has been discussed.

Inelastic collisions among grains lead to qualitative differences from the dynamics of normal fluids (e.g., large scale instabilities). The effects of such inherent energy loss have been studied at both the Liouville and Boltzmann kinetic theory levels. The experience gained here will be exploited in future research on confined, charged dust particles.

Collaborators, Postdocs, Students

Collaborations on this NSF/DOE research have been possible by leveraging limited grant funds. One graduate student (Aparna Baskaran, PhD May 2006) and has received support from the grant but with significant local support through competitive awards from the University of Florida. A second student under the direction of collaborator Bonitz (Andrea Fromm, Ms. December 2006) was supported by the University of Kiel. Postdoctoral fellow Yannick Marandet received half of his support from the French government. Postdoctoral fellow Jeff Wrighton has contributed without funding from this grant. Visitor Michael Bonitz, Professor of Physics, University of Kiel (Germany) was primarily supported by the grant. The PI's continued collaboration with the University of Provence is supported by the French government.

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