The objective of the research “Correlations in Confined Quantum Plasmas” under NSF-DOE Partnership Grant DE FG02 07ER54946 was to understand strong correlations among charged particles in the presence of both confinement and quantum effects. Examples of such confined systems of current interest include ultra-cold plasmas in a trap, valence electrons in metallic clusters, and electrons in quantum dots. The general properties of interest are those related to the thermodynamics, structure, and dynamics of the charged particles. The methods used were both theoretical and computational, guided by the new and evolving results from experimental investigations.

Effective potentials for classical many-body methods

In addition to purely quantum methods (e.g., path integral Monte Carlo (PIMC) for simulation; Green’s functions for theory), powerful classical methods (e.g., molecular dynamics simulation; liquid state theory) can be adapted for applications to quantum systems using effective potentials. Although this idea is quite old, its implementation has typically been limited to weak coupling diffraction effects. This method was utilized to illustrate the combined effects of diffraction and degeneracy for an impurity in a degenerate Fermi gas. A systematic mapping of a quantum system to a representative classical system for equilibrium states is part of the proposed research here.

In a different direction, effective potentials appropriate for non-equilibrium states were studied. One approach was based on non-equilibrium Green’s functions (NEGF). The equation for the spectral density was simplified by introducing a classical form for the kinetics, and nonlocal quantum effects were accounted for by replacing the bare external confinement potential with an effective quantum potential. A quantum kinetic theory of trapped particles in a strong electromagnetic field was obtained in this way.

The dynamics of strongly correlated ions in a partially ionized quantum plasma was described by coupled equations for the ion and electron reduced density operators. A dynamical mean field approximation was introduced to allow a classical description of strongly coupled ions with dynamical screening by the electrons. The effect on the ions of the electron dynamics, electron streaming, and wake effects, was studied.

An application of the regularized electron – ion potential to the dynamics of electrons about an impurity ion was considered. The resulting classical kinetic theory for the electrons was used to show the dominant role of bound states for large charge number. The relevance for plasma spectroscopy and ion stopping was noted.

Coulomb Balls and Shell Structure

Prior to the start of this award, the group at CAU was already studying the lowest energy states for charges in a harmonic trap via analytic shell models, molecular dynamics (MD) and Monte Carlo (MC), and path integral Monte Carlo (PIMC) simulations. During the grant period complementary tools based in liquid state theory were developed to describe the formation of shell structure as a function of temperature over the entire fluid phase. Detailed comparisons with Monte Carlo simulations were performed showing remarkable agreement for the number of shells, their location, and occupation numbers. Ongoing work is directed at extending this formalism to the prediction of Wigner crystallization (charge localization within the shells). The classical description of strong coupling and confinement through theory and simulation is now quite complete.

Photoionization Processes in Atoms

Strong correlation effects in finite quantum systems were studied for few-electron atoms (real atoms where confinement is imposed by the Coulomb potential of the nucleus). The main goal was to describe the time-dependence after femtosecond excitation by a laser pulse, using non-equilibrium Greens functions and wave function based approaches. The multiconfiguration time-dependent Hartree-Fock (MCTDHF) method has been applied to a model one-dimensional atom with up to four electrons. The ground state energies and the time-dependent photoionization by the field of a strong laser pulse with two different frequencies in the ultraviolet were calculated. The first full 3D MCTDHF results have now been obtained.

Collaborators, Postdocs, Students

The award did not provide support for postdoctoral / research fellows. Nevertheless two fellows had active participation in this program: Alexei Filinov at CAU and Jeff Wrighton at UF. Partial support for two graduate students was provided. Dufty and Bonitz converted all of their salary / consultant fees for additional graduate student funds. Christian Henning was awarded the prize for best theory PhD thesis of Kiel Physics Department 2009 and the prize for best thesis of the College of Mathematics and Natural Sciences of Christian Albrechts Universität 2009. Other students receiving partial support were Patrick Ludwig and David Hochstuhl at CAU, and Sandipan Dutta at UF. During the grant period, the Bonitz group organized two summer schools in the US and Germany. They also presented a mini-course on computational methods to the UF condensed matter students via video telecast.

Presentation of results

In addition to the 19 refereed publications listed below, results of this research were presented as invited lectures and contributed posters at several international conferences, professional society meetings, workshops, and summer schools: APS Plasma Meeting, November 2007; International Conference on Spectral Line Shapes, Spain, June 2008; Strongly Coupled Coulomb Systems, Italy, July 2008; Frontiers of Quantum and Mesoscopic Thermodynamics, Czech Republic, July 2008; Graduate Summer Institute, *Complex Plasmas,* August 2008, Hoboken N.J.; Annual Plasma Physics Conference of the German Physical Society, March 2009; Complex Systems of Charged Particles, Moscow, April 2009; Progress in Nonequilibrium Greens functions IV, Glasgow, August 2009. Physics of Nonideal Plasmas, Moscow, September 2009; Modern Problems of Theoretical and Mathematical Physics, Kiev, September 2009; APS Plasma meeting, Atlanta, November 2009; APS March meeting 2010; German Physical Society, Düsseldorf, March 2010; Graduate Summer Institute "Complex Plasmas", August 2010, Greifswald, Germany; International Conference on Interplay of Electronic Structure Theory and Experiment, Sandbjerg, Denmark, July, 2010; 51st Sanibel Symposium, St. Simons, Georgia, February, 2011; APS March Meeting, Texas, March, 2011; Strongly Coupled Coulomb Systems, Budapest, July 2011; Frontiers of Quantum and Mesoscopic Thermodynamics, Prague, Czech Republic, July 2011; "Strongly Coupled Ultra-cold and Quantum Plasmas", Lisbon, Portugal, September 2011; ITER-IAEA-ICTP Advanced workshop on Fusion and plasma science, Trieste, Italy, October 2011

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