Clusters and Phase Transitions

Conference

Magnus Haus
Berlin, Germany
10. - 12. October 1996

Welcome

Welcome to Berlin, welcome to the Conference "Clusters and Phase Transitions", which is dedicated to recent developments in statistical physics. The invited lectures will present the topic from various perspectives, ranging from nuclear matter to biophysics.

We grateful acknowledge financial support by the the Alexander von Humboldt Foundation (Bonn). During the conference, fellows of the Humboldt Foundation and German Scientists, working in the field of plasma physics, thermodynamics and phase transitions, have the opportunity to meet with two laureates of the Humboldt Research Award, Prof. S. Ichimaru (Tokyo) and Prof. Yu. L. Klimontovich (Moscow).

Our conference center, the historical "Magnus Haus", owned by the Deutsche Physikalische Gesellschaft, is a reknowned meeting place for physicists in Berlin. The house was build already in 1760, it is named after the famous German physicist Gustav Magnus, who owned the house in the mid 19th century and established here the first Physical Institute in Germany.

Located in the heart of the city, directly on the Spree River and right across the world-famous Pergamon Museum, the Magnus Haus offers the best facilities for our small conference, suitable both for an intensive exchange of ideas and relaxed discussions in the backyard during the breaks. The personal atmosphere at this small conference should provide ample possibilities to to renew long-lasting contacts and to establish new ones.

Best wishes for an interesting and stimulating conference and a pleasant stay in Berlin.

Lutz Schimansky-Geier Frank Schweitzer

Program

Thursday, 10. October	
14.00	**Opening of the conference**
14.15	Yu. L. Klimontovich (Moscow) Thermodynamic and Kinetic Description of the Second Order Phase Transitions
15.30	*Coffee Break*
16.00	W. Ebeling (Berlin) Quantum Statistics of Plasma Phase Transition
16.45	G. Röpke (Rostock) Tentative Title: Phase Transitions in Nuclear Matter
17.30	*Break*

Program

Friday, 11. October	
09.30	F. Hensel (Marburg) Phase Transitions in Fluids that Exhibit Changes in Electronic Structure
10.15	D. Kremp, Th. Bornath, M. Bonitz (Rostock) Quantum Kinetic Equations, Memory Effects, Conservation Laws
11.00	*Coffee Break*
11.30	W. Muschik (Berlin) Jump Conditions and Second Law at Phase Interfaces
12.15	D. Lohse, S. Großmann (Marburg) Sonoluminescence: Why the Fiery Bubble has Eternal Life
13.00	*Lunch and Coffee Break*
15.00	Yu. Romanovsky (Moscow) Stochastic Cluster Dynamics of Macromolecules
15.45	F. Schweitzer (Berlin) Cluster Formation Simulated by Active Brownian Particles
16.30	L. Schimansky-Geier (Berlin) Non-Equilibrium Phase Transitions
17.15	*Break*

Program

Saturday, 12. October	
9.45	S. Ichimaru (Tokyo) Phase Transitions in Astrophysical Dense Matter
11.00	*Coffee Break*
11.30	A. Förster (Berlin) The Equation of State of Dense Plasmas
12.15	W.D. Kraeft, J. Riemann, M. Schlanges (Greifswald) Thermodynamics of Strongly Coupled Plasmas
13.00	**Closure of the Conference**

Quantum Statistics of Plasma Phase Transition

W. Ebeling

Institute of Physics, Humboldt University, Berlin, Germany

A survey on the theoretical predictions of plasma phase transitions is given.

First a simple analytical theory for charge-symmetrical systems based on Debye-Huckel-type approximations is developed. Several generalizations taking into account quantum statistical effects in a more precise way, e.g. by Pade approximations are discussed.

The location and the properties of the critical point are discussed for several special plasmas. Finally a comparision of the Pade approximations with recent data from Monte Carlo calculations and from quantum molecular dynamics is given.

The Equation of State of Dense Plasmas and the Plasma Phase Transitions

A. Förster

Institute of Physics, Humboldt University, Berlin, Germany

The equation of state, the ionization and dissociation equilibrium of dense plasmas are determined by the complex interplay of the statistics of the plasma particles, of the Coulomb interaction between the charges, as well as of the quantum–mechanical exchange. The chemical picture which introduces the different bound states of nuclei and electrons as new elementary plasma constituents has paved the way for several sophisticated models for the thermodynamic properties of dense plasmas developed over the last 30 years.

The so–called "plasma phase transition", a first–order phase transition in partially ionized plasmas, accompanied by a discontinuity in the ionization state, was theoretically predicted by different groups starting with the works of Norman and Starostin (1968) and Ebeling and Sändig (1973).

The proposed talk aims at a review and comparison of recent results from the 90's concerning chemical models for hydrogen, helium, carbon, and their mixtures, experimental data from shock-wave compression and numerical simulations based on the path–integral Monte Carlo method.

Sonoluminescence: Why the Fiery Bubble has Eternal Life

D. Lohse, S. Großmann

Department of Physics, Philipps University, Marburg, Germany

Sound driven gas bubbles in water can emit light pulses. This phenomenon is called sonoluminescence (SL). Two different phases of single bubble SL have been proposed: diffusively stable and diffusively unstable SL. Phase diagrams are presented in the gas concentration vs forcing pressure state space and also in the ambient radius vs forcing pressure state space.

These phase diagrams are based on the thresholds for energy focusing in the bubble and on those for (i) shape instabilities and (ii) diffusive instabilities. Stable SL only occurs in a tiny parameter window of large forcing pressure amplitude $P_a \sim 1.2 - 1.5$ atm and low gas concentration of less than 0.4% of saturation.

The results quantitatively agree with experimental results of Putterman's UCLA group on argon, but not on air. However, air bubbles and other gas mixtures can also successfully be treated in this approach if in addition (iii) chemical instabilities are considered.

The essential feature is the removal of almost all nitrogen and oxygen from the bubble through reaction to soluble compounds (i.e. NO_x or NH_3). – We also discuss possible applications of bubble dynamics in medicine.

Phase Transitions in Fluids that Exhibit Changes in Electronic Structure

F. Hensel

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The vapour phase of fluid metal is distinct from that of normal insulating fluids such as argon in that its electronic structure and interparticle interaction is strongly depending on density. The most striking manifestation of this density dependence is the nonmetal to metal transition which shows up when a metal vapour is compressed to the region of the liquid–vapour critical point.

The lecture discusses recent experimental results in the liquid–vapour critical region of metals which show that the existence of the metal–nonmetal transition noticeably influences the electronic, thermodynamic, structural, dynamic, and interfacial features of fluid metals. In particular, we examine the density–dependent metal–nonmetal transition for the Group 1 elements hydrogen, caesium and rubidium.

The main emphasis is on the depolarized interaction induced light scattering spectrum of mercury vapour as a function of density and temperature and on optical reflectivity experiments on mercury against an optically transparent substrate close to the vapour–liquid coexistence curve. The temperature- and density dependence of the reflectivity reveals clearly the existence of a prewetting transition of mercury on the sapphire substrate. The transition line, which terminates at hight temperature at a surface critical temperature T_{sc}, lying below the bulk critical temperature T_c and at low temperature at the wetting transition temperature T_w, lies close to the bulk vapour–liquid coexistence curve and occurs when the bulk vapour pressure is within a few percent of its value at saturation.

Phase Transitions in Astrophysical Dense Matter

S. Ichimaru

Department of Physics, University of Tokyo, Japan, *and*
Max-Planck Institute for Quantum Optics, Garching, Germany

In this lecture, I wish to describe recent progress in the theories of phase transitions in systems of fermions, such as electrons, protons, neutrons, and helium-3. Meant by "phase transitions" here are gas- liquid transition, liquid-solid transition, ferromagnetic transition, and insulator-to-metal transition. Phase boundaries between paramagnetic and ferromagnetic states and those between fluid and solid states in Fermi liquids with repulsive interaction are calculated by evoking a correspondence-of-states argument; a phase diagram calculated for electron liquids is thus extended to that for liquid-metallic hydrogen as well as to those with hard-core repulsion such as liquid helium-3 and neutron liquids.

It is shown through comparison with observed data that the ferromagnetic transitions may be relevant to the mechanisms for magnetic dwarf stars; the physical conditions for realization of a ferromagnetic state may be expected across a shell domain in an outer hydrogen layer of a white dwarf and in an inner crust of a neutron star. Possibility of laboratory realization for nuclear ferromagnetism in a dilute cryogenic system of helium-3 is elucidated.

Phase diagram of hydrogen matter describing the states arising from combinations between molecular, atomic, metallic, solid, liquid, gaseous, and/or ionized realizations of the matter is obtained, capable of qualitatively reproducing the phase information that we know through terrestrial experiments; it can cover the phases in the parametric regime: $1 <= P(bar) <= 10^8, 20 <= T(K) <= 10^6, 10^-4 <=$ mass density $<= 10$. The results of recent Livermore experiment on metallization and electric conductivity, using a shock wave reverberating between electrically insulating sapphire anvils to compress hydrogen to pressures of 93-180 GPa, are analyzed in light of the phase diagram and theories of the conductivities. Possible implication of the phase diagram in accounting for Jovian excess infrared luminosity is remarked.

Thermodynamic and Kinetic Description of the Second Order Phase Transitions

Yu. L. Klimontovich

Department of Physics, M.V. Lomonossov Moscow State University, Moscow, Russia

Thermodynamic and kinetic description of phase transitions for the model of ferroelectrics on a basis kinetic equation for the distribution function of values of the "order parameter", coordinates and time is considered.

For one-domain ferroelectrics the self-consistent approximation for the first moment is used. The kinetic equation is reduced to the relaxation Ginsburg-Landau equation. The susceptibility is governed by the Curie law and the heat capacity has the jump.

Calculations are carry out and for polydomain ferroelectrics. In this case the self-consistent approximation for the second moment is used. In the last case there is the jump of the susceptibility. The heat capacity governed by the Curie law.

The calculation of fluctuations of the first and the second moments are carry out for all temperatures for switching on and at the critical point.

It is shown also that the Ornstein-Zernike formula has the place not for the space correlator of fluctuations, but it is valid only for the time spectral density of the space correlator at zero frequency.

In the kinetic theory of the phase transition all physical characteristics in the critical point have finite values. Thus the problem of the "infinities" is absent.

Thermodynamics of Strongly Coupled Plasmas

W.D. Kraeft, J. Riemann, M. Schlanges

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Greifswald, Germany

In the framework of Green's functions, general expressions for thermodynamic functions of plasmas are presented. The low density limit is discussed in detail. Especially, the exact expression up to the second order (second virial coefficient) is given. These terms include contributions of bound states, which are collected in the Planck-Larkin sum of bound states.

The question of compensation between bound and scattering states is discussed. The next order contributions $n^{5/2}$ are determined. Our analytical results are compared with quantum Monte-Carlo data.

Quantum Kinetic Equations, Memory Effects, Conservation Laws

D. Kremp, Th. Bornath, M. Bonitz

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In the framework of real-time Green's functions, a general non-Markovian Boltzmann equation including initial correlations, full time retardation (memory) and self energy is considered. This equation conserves the total (kinetic plus potential) energy.

Two approximations of this very general equation are investigated: (i) the first order expansion with respect to the retardation and (ii) the first Born approximation for the scattering T-matrix (non-Markovian Landau equation).

The influence of memory and damping effects on the relaxation of the one-particle distribution and of the kinetic energy is demonstrated by a numerical analysis. The results of the kinetic equation are compased with the resukts from the two time Kadanof-Baym equation.

Jump Conditions and Second Law at Phase Interfaces

W. Muschik

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Tentative Title: Phase Transitions in Nuclear Matter

G. Röpke

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Stochastic Cluster Dynamics of Macromolecules

Yu. Romanovsky

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Since the known paper of L. Pontryagin, A. Andronov and A. Vitt (1933) a lot of problems were considered in nonlinear dynamics, associa- ted with the study of the transition of a multistable system from one stable state to another under the influence of noise. In the recent years new problems emerged in the studies of complex vibrational systems. These problems deal with the transitions of a test particles (TP) in the 2D potential relieves with the fluctuating or periodically changing pa- rameters.

As a complex relief is a variant of Sinai billiard, the motions of TP therein become stochastic even without any external action. The examples of the cluster dynamics of macromolecules are considered. The dependencies are established of the time of transition of a TP from the area of one minimum to the zone of attraction of another one on the frequency of the periodic changes of the parameters of the potential relief. The finite sizes and shape of TPs are taken into account. The problem of quasi-solitons moving in nonhomogenious branching chains is of our interest too. The study of these processes will alow us to get closer to the comprehension of principles of molecular machines.

Reference:

Ebeling W. , Romanovsky Yu., Khurgin Yu., Netrebko N., Netrebko A., Shidlovskaya E.: Complex regimes in the simple models of the molecular dynamics of enzymes. In: Proc. SPIE , vol. 2370, 1994. 5th Inter. Confer. Laser Application in Life Sciences (LALS-94) 1994. pp. 434-447.

Non-Equilibrium Phase Transitions

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Cluster Formation Simulated by Active Brownian Particles

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Active Brownian particles are Brownian particles with the ability to generate a self-consistent field, which in turn influences their further movement and physical and chemical behavior. This non-linear feedback between the particles and the field generated by themselves results in an interactive structure formation process, which, on the macroscopic level in most cases can be described by sets of coupled reaction-diffusion equations.

The main idea of our approach is to solve the LANGEVIN equations for an ensemble of active Brownian particles instead of the related nonlinear partial differential equations (PDE). Our approach provides a quite stable and fast numerical algorithm for simulating processes even for large density gradients and is applicable also in cases where only small particle numbers govern the structure formation.

In order to demonstrate the applicability of our approach, we first investigate biological aggregation processes based on chemotactic response. Further, the model will be extended by considering internal degrees of freedom for the active Brownian particles. As an application, the formation of urban clusters is discussed.