The 3-rd Conference

Statistical Physics: Modern Trends and Applications

23–25 June 2009, Lviv, Ukraine

Dedicated to the 100-th anniversary of Prof. M.M. Bogolyubov (1909–1992)

BOOK OF ABSTRACTS

Lviv – 2009

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The 3-rd Conference "Statistical Physics: Modern Trends and Applications" will be held in June 23–25, 2009, in Lviv, Ukraine. It is organized by the Institute for Condensed Matter Physics (Lviv, Ukraine) and is dedicated to the 100-th anniversary of Academician M.M.Bogolyubov (1909–1992) and to the 40-th anniversary of the Department of Statistical Theory of Condensed States of Institute for Theoretical Physics (Kyiv), which formed the basis of the Institute for Condensed Matter Physics.

The Conference will be organized in the form of invited lectures (about 30 min), contributed talks (about 20 min) and poster presentations. Official language of the Conference is English.

Main topics

- Quantum many-particle systems
- Soft condensed matter
- Cooperative phenomena and phase transitions
- Non-equilibrium and transport phenomena
- Surface phenomena
- Exotic problems of statistical physics

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Bound states of electrons with soliton-like excitations in one- and two-dimensional thermal systems

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We study the excitation of solitons in atomic systems with Morse interactions one-dimensional chains and planar samples in the region from low to intermediate temperatures and their influence on electrons moving in the lattice. The atoms are treated by classical Langevin equations for particles with Morse interactions. The dynamics of the free electrons is modelled in the framework of the tight binding model using Schrödinger and Pauli master equations. It is shown that electrons may form rather stable bound states with soliton-like excitations, an effect which was first detected by Davydov. We study the excitations of these quasiparticles, which move in general with supersonic velocity and are called here solectrons, in dependence on the temperature. Transport properties in particular diffusion are described by time-correlations and Kubo-type expressions. Several applications in particular to biopolymers are discussed.

Entropy driven mechanism for ordering, phase separation and patterning in binary stochastic systems

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We have studied phase transitions in extended systems, wherein the ordered phase only results if a randomly fluctuating source is introduced into the dynamical system. We consider ordering processes in systems with internal noise with intensity dependent on the field variable. It was shown that phase transformation observed in systems with conserved and non-conserved dynamics are of entropy driven mechanism when the ordered phase appears due to the balance between the relaxing forces moving the system to the homogeneous state, and field-variable dependent fluctuations pulling the system away from the disordered state.

Considering entropy-driven phase transitions in systems with non-conserved dynamics it was shown that in the case of symmetrical local potential reentrant phase transitions can be observed. In systems with an asymmetric local potential phase transitions display hysteresis-like behavior of the order parameter. Considering phase separation processes in stochastic systems with a field dependent kinetic coefficient and an internal multiplicative noise it was found that dynamics of spinodal decomposition at early and late stages essentially depends on the field dependent mobility. It was shown that internal fluctuations lead to slowing down kinetics of domains growth. A mean field approach was carried out in order to obtain the stationary probability, bifurcation and phase diagrams displaying reentrant phase transitions. It was shown that phase separation scenario is determined by entropy driven mechanism. We have studied the entropy-driven mechanism leading to stationary patterns formation in stochastic systems with local dynamics and non-Fickian diffusion. It is shown that a multiplicative noise is able to induce and sustain stationary structures. It was found that at small and large noise intensities the system is characterized by unstable homogeneous states. At intermediate values of the noise intensity three types of patterns are possible: nucleation, spinodal decomposition and stripes with liner defects (dislocations).

Properties of phase separation processes in binary stochastic systems with thermal diffusion and ballistic mixing

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We have considered dynamics of binary stochastic systems with thermal diffusion and ballistic mixing representing irradiation influence. Starting from the continuity equation for the concentration field we have obtained the Langevin equation describing behaviour of globally conserved quantity with thermal diffusion flux and ballistic mixing term describing fluctuating environment (atom relocation due to irradiation). Introducing fluctuations of thermal flux and a source representing regular and random atom relocations we have shown that there are two competing mechanisms of phase transitions: thermally assisted diffusion and irradiation induced atomic exchange. In our model ballistic mixing leads to atomic exchange to nearest, next and next-next neighbors of the fixed atom.

We have studied dynamics of the structure function at early stages of spinodal decomposition. It was shown that with an increase in the regular part of ballistic mixing describing nearest atomic neighbors a critical wave-vector values are decreased. An increase in the correlation radius of atomic jumps leads to decrease in the domain of the system parameters where unstable modes growth. In the framework of the mean field theory we have derived the effective Fokker-Planck equation to describe phase separation processes in systems with ballistic mixing and thermally activated diffusion. It was found that changing the composition in a binary alloy a domain of ordered phase decreases when ballistic mixing intensity and temperature increase. A reentrant behavior of the mean field order parameter was found versus the intensity of stochastic part of ballistic mixing term. Considering macroscopic approximation it was found that except ordinary phase separation processes a patterning is realized. With increase in the ballistic mixing strip patterns are realized. Phase separation processes and patterns formation are studied in details.

Statistical properties of the ballistic deposition and solid on solid models

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The study of the statistical property of surfaces growing under the deposition of particles has helped researchers to find new information about surfaces. The theoretical description are based on continuous models: the Edwards-Wilkinson model, the Kardar-Parisi-Zahang(KPZ) equation and models based on molecular beam epitaxy. The focus of this study has been statistical characterization of the growing surface. This is achieved by simulating ballistic deposition and restricted solid on solid models. We found same roughness and growth exponent as they are in a same universality class(KPZ). In our investigation we have found some different properties for those. We determined Markov property, Markov length scale and Keramers-Moyal coefficients. These two models can be distinct by differences between them.

Molecular theory of hydrodynamic boundary conditions in nanofluidics

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We propose the first-ever statistical-mechanical derivation and calculation of the hydrodynamic slip length. Our approach is based on combination of linear response theory and equilibrium molecular theory of solvation. The slip length derived is related to the fluid organization near the solid surface, as governed by the solid-liquid and liquid-liquid interaction. In the wide range of shear rates and surface-liquid interactions, the slip length is expressed in terms of the Green-Kubo-Nakano relations as a function of the anisotropic inhomogeneous time correlation function of density fluctuations of the liquid in contact with the surface. The time dependence of the correlation function is factored out by treating it in the hydrodynamic limit. The spatially inhomogeneous two-body correlation function is represented in the Kirkwood-like approximation as a product of the three-dimensional density distributions of interaction sites of the liquid near the surface and the site-site pair correlations of the bulk liquid. The presented treatment generalizes the phenomenological definition of the friction coefficient (as well as the slip length) to a tensor quantity, which reflects an anisotropic nature of an ordered crystalline or nanopatterned surface. This enables theoretical prediction of friction forces acting aslant to the liquid flow direction for such surfaces. We derive generic analytical expressions for the liquid-surface friction coefficient (and slip length) for an arbitrary surface-liquid interaction potential. We further illustrate it by numerical calculations for a laminar flow of nine different molecular liquids at ambient conditions in contact with the (100) FCC surface of gold, copper and nickel modeled by using OPLS models for liquids and the Steele potential for crystalline surfaces. The obtained values for slip length range from few to hundreds of nanometers and microns, and are consistent with experimental measurements.

Flux periodicities in loops of nodal superconductors

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The magnetic flux periodicity of superconducting loops as well as flux quantization itself are a manifestation of macroscopic quantum phenomena with far reaching implications. They provide the key to the understanding of many fundamental properties of superconductors. In superconducting rings the electrical current has been known to periodically respond to a magnetic flux with a periodicity of $hc/2e$. The $hc/2e$ periodicity is viewed to be a hallmark for electronic pairing in superconductors and is considered evidence for the existence of Cooper pairs. Here we show that in contrast to this long-term belief, rings of many superconductors bear an hc/e periodicity instead. For nodal superconductors, the flux induced Doppler shift of the near-nodal states leads to a flux dependent occupation probability of quasi particles circulating clockwise and counter clockwise around the loop, which results in am hc/e periodic component of the supercurrent, even at zero temperature. We analyze this phenomenon in an analytic approach and also numerically—both within the framework of conventional BCS theory. Specifically for d-wave pairing, we show that the hc/e periodic current component decreases with the inverse radius of the loop.

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Towards thermodynamics of flat-band electron systems

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The standard N-site repulsive Hubbard model with the Hamiltonian

$$H=\sum_{\sigma=\uparrow,\downarrow} H_{0\sigma}+H_U, H_{0\sigma}=\sum_{\langle i,j\rangle} t_{ij}\left(c^{\dagger}_{i\sigma}c_{j\sigma}+\text{h.c}\right), H_U=U\sum_i n_{i\uparrow}n_{i\downarrow}$$

is among simplest models of strongly correlated systems, although rigorous analysis of its properties is a difficult task. In the early 90s A. Mielke and H. Tasaki, while studying the origin of ferromagnetism in intinerant electron systems, considered a class of lattices, which have a special property that the lowest-energy one-electron band is completely dispersionless (flat), and proved rigorously the existence of ferromagnetism in this class of Hubbard models at zero temperature and certain electron filling factors (for review see [1]). Later on, low-temperature thermodynamics of the Hubbard model on some of these lattices was obtained rigorously around a particular value of the chemical potential μ_0 [2].

The aim of the present paper is to examine a region of validity of the method used in [2], i.e. to estimate until which particular (low) temperature and within which particular chemical potential region (around μ_0) the elaborated in [2] approach does work. To achieve this goal we consider some one-dimensional lattices, which support the lowest-energy flat one-electron band (sawtooth and two kagomé chains), assume $U=0$, adopt a grand-canonical description, and perform *i)* exact calculation of thermodynamic quantities in a whole half-plane chemical potential μ – temperature $T>0$ and *ii)* calculation of thermodynamic quantities using the method suggested in [2]. Comparing both results in the μ – T half-plane we discuss in detail to what extent the approach of [2] reproduces exact results in noninteracting limit. Our analysis refers to the entropy, specific heat, and the average number of electrons.

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2. O. Derzhko, A. Honecker, and J. Richter, Phys. Rev. B **76**, 220402(R) (2007); *ibidem* **79**, 054403 (2009).

Quantum statistical theory of submonolayer magnetic films at simple metal surfaces

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Ultrathin and submonoatomic magnetic films have well perspective in applying as basic elements of magnetic sensors, spintronics, micro- and nanoelecrtonics. Today there are many principal theoretical and experimental problems, particularly, conditions of surface magnetism or co-existence magnetic phase of films. We propose microscopic model of submonoatomic film, adsorbed at crystal surface of simple metal. Besides, model Hamiltonian takes into account exchange interactions and resonance electronic transfer "film – semi-bounded metal". Electron states of adsorbed magnetic film are investigated by means of functional integration method.

Functional integral theory of chemisorption

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The microscopic model of chemisorption for hydrogen-like atoms at simple metal surfaces is generalized. The functional representation of the thermodynamical potential and the temperature Green functions are obtained. Some specific approximation schemes for calculation of the functional integrals are discussed. The method of functional integration is proposed to study the exchange and correlative interaction in the scope of quantum theory of chemisorption for hydrogen-like atoms. Charged and magnetic states of hydrogen at simple metal with square surface lattice are calculated.

The relativistic electrodynamics least action principles revisited: new charged point particle and hadronic string models analysis

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The work is devoted to studying some new classical electrodynamics models of interacting charged point particles and related with them the quantization via Dirac procedure aspects. Based on the vacuum field theory no-geometry approach, developed by authors in [2,3], the Lagrangian and Hamiltonian reformulations of some alternative classical electrodynamics models are devised. The Dirac type quantization procedure for the considered alternative electrodynamics models, based on the obtained canonical Hamiltonian formulations, is developed. The classical relativistic least action principle [1] is revisited from the vacuum field theory approach and analyzed in detail. New physically motivated versions [2-4] of relativistic Lorentz type forces acting on a point charged particle are derived, a new relativistic hadronic string model is proposed and analyzed in detail. New string dynamic equations with distributed mass and charge densities are obtained with respect to the proper reference system time parameter.

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Entangled-like chain dynamics in polymer mixtures of non-entangled chains

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We present molecular dynamics simulations on a simple model for polymer blends. The selected values for the chain length N are in all cases much smaller than the entanglement length of the corresponding homopolymer. At odds with standard predictions of the Rouse model, the increase of the dynamic asymmetry between the two components in the blend induces strong non-exponential behaviour for the Rouse normal modes of the fast component. From simple scaling arguments we infer that strong non-exponentiality is an intrinsic feature which does not arise from a simple distribution of elementary exponential processes. Despite simulated chains being much shorter than the entanglement length, strong dynamic asymmetry induces dynamic features, as anomalous scaling properties for the Rouse modes, resembling observations in strongly entangled homopolymers.

This unusual behavior is associated to strong memory effects which break down the assumption of time uncorrelation of the external forces acting on the tagged chain. The observed anomalous scaling laws for the Rouse modes strongly resemble predictions from recent theoretical approaches based on generalized Langevin equations (GLE). Within the approach of renormalized Rouse models for the memory kernel, anomalous scaling of the Rouse modes is directly connected to slow relaxation of density fluctuations around the tagged chain. The latter may be induced by entanglement, but data reported here for the fast component suggest that this is not a necessary ingredient. Analogies with entangled-like dynamics are indeed observed even for $N = 4$ monomers, provided that dynamic asymmetry in the blend is sufficiently strong. In summary, results presented here suggest a more general frame, beyond the usual reptation picture, for chain relaxation features usually associated to entanglement effects. They also open new possibilities for the application of GLE methods in complex polymer mixtures.

Molecular dynamic simulations of concentrated solutions for Lithium-ion batteries

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For the mean time the propylene carbonate (PC) – dymethoxyethane (DME) mixed solvent is considered as an appropriate system for modelling the microscopic structure and ion dynamics in the electrolyte solutions based on cyclic carbonates, linear esters and lithium salts.

In the present work effective force field models of PC and DME molecules were developed for molecular dynamics (MD) simulations of $LiBF_4$ solutions based on PC–DME mixtures. PC and DME molecules were represented by a six-site unpolarizable flexible and a seven-site unpolarizable rigid models, respectively. Partial atomic charges, molecule geometries and dihedral potentials for DME molecule were obtained by quantum-chemical calculations in the media at the B3LYP/aug-cc-pVTZ level of theory in the framework of the reaction field model of the surrounding media.

The MD simulations were performed for pure solvents and their mixtures with a PC molar content of 25%, 50% and 75%, and infinitely diluted, 0.1 M and 1.0 M $LiBF_4$ solutions in these mixtures. The validation of the proposed force field models was done by the comparison of the experimental and calculated limiting molar conductivities (λ_0^i) of the Li^+ and BF_4^- ions.

It was found that Li^+ solvation shell consists of six PC molecules for all the systems under the question excluding pure DME, where the coordination number was found to be equal to six due to the three DME molecules within the first solvation shell.

It was also found that in 0.1 M mixtures the Walden product doesn't depend on the mixed solvent composition ($\lambda_0^i \cdot \eta = \text{const}$) due to a preferential solvation of Lithium cation by six PC molecules.

For 1.0 M $LiBF_4$ solutions in PC special attention paid to the MD simulation of systems with different initial configuration of the ionic subsystem, and to the influence of the association degree on the viscosity and conductivity of electrolyte solutions.

Diffusion coefficient of macroradicals in polymer matrix

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Evaluation of macromolecules diffusion coefficients in polymer matrix is of a great scientific and practical interest, however, it is sufficiently complicated experimental task since many properties (in particular, the elastic ones) of polymer matrices are affected by the macromolecules conformation thermodynamics that determines their equilibrium elastic characteristics as well as by macromolecules conformation ability to react quickly or slowly upon external disturbances, that is by kinetic factors. Dynamics of macromolecules deformation and their transmission mobility are based on the general reptilian mechanism which is realized by segmental mobility of polymer chain links.

In the presented work diffusion coefficient of macroradicals in 1,6-hexanediolbiacrylate matrix was numerically evaluated by ESR-spectroscopic method of the analysis of macroradicals decay kinetics within the temperature interval of $45 \div 80^o$C. It was found that kinetics of macroradicals decay can not be described in the second order reaction coordinates, what is typical for quadratic chain termination. Kinetic equation, which satisfactorily describes experimental data, was obtained. On the assumption that it is connected with macroradicals propagation till their meeting and decay the kinetic equation, which satisfactorily describes experimental data, was obtained. This equation allows to obtain the numerical values of the quadratic chain termination rate constant. Using these values as well as the Smolukhovsky equation the numerical values of the macroradicals diffusion coefficients were obtained in the given temperature interval $D = (2.7 \div 31) \cdot 10^{-19}\mathrm{m}^2/\mathrm{s}$, the characteristic times of the polymer chain links segmental motion $\tau = (10 \div 1) \cdot 10^{-5}\mathrm{s}$, their activation energy ($E = 76.3\mathrm{kJ/mol}$) and entropy ($\Delta S/R = 8.3$) were estimated. Hence, high values of τ (by 4 - 5 order more than in solutions) determine low values of the macromolecules diffusion coefficients in polymer matrices and, respectively, considerable effect of kinetic factors on their properties.

Distribution of internal links of the polymer chain in self-avoiding random walks statistics

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Within the frame of self-avoiding random walks (SARW) statistics the derivation of the internal n-link ($1 \ll n \ll N$) distribution of the polymer chain regarding to the chain ends is offered. The analysis of the obtained expressions shows that the structure of the conformational volume of the polymer chain is heterogeneous; the largest density of the number of links takes place in conformational volumes nearby the chain ends. It can create the effect of the blockage of the active center of the growing macroradical and become apparent as linear chain termination. The equation for the most probable distance between two internal links of the polymer chain was obtained as well. The polymer chain parts, separated by fixing of the internal links, are interactive subsystems. Their total conformational volume is smaller than the conformational volume of the undeformed Flory ball. Respectively, the total free energy of the conformation of the chain parts is equal to the free energy of the conformation of the deformed (i.e. compressed till the total volume of the chain parts) Flory ball.

Electron transport in strongly anisotropic structures in a magnetic field

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The linear response of electron system of a layered conductor to the presence of a temperature gradient and an electric field is investigated theoretically at temperature which is much below than the Debye temperature T_D. We consider thermoelectric effect in a Q2D conductor with several groups of charge carriers that are responsible for the electron transport. The Fermi surface in such conductor may consist of topologically different elements: weekly corrugated cylinders and planes. In the range of very low temperatures the relaxation in electron system of a degenerated conductor is realized mainly by charge carriers scattering at impurity centers and other crystal defects. This is the case when the momentum relaxation time τ_p and the energy relaxation time τ_ε are of the same order of magnitude. At higher temperatures an extra mechanism of charge carriers relaxation, connected with the electron scattering by crystal lattice vibrations, leads to decreasing of the relaxation times with T increasing, and τ_ε decreases more slowly than τ_p does. In the absence of a magnetic field the temperature dependence of the thermoemf has a maximum when both of the mechanisms of the electron relaxation are comparable. We have shown that in a strong magnetic field competition of different mechanisms of charge carriers relaxation gives rise to various T-dependencies of the thermoelectric field. The presence of the plane sheet of the Fermi surface affects essentially the behavior of the thermoemf and its T-dependence may have a minimum at certain orientation of the vectors $\mathbf{B}$ and ∇T. The experimental study of thermoelectric effect is shown to be a very convenient method for determining the structure of charge carriers energy spectrum and different relaxation mechanisms in the system of conduction electrons.

High-frequency impedance of layered conductors in a quantizing magnetic field

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The propagation of electromagnetic waves in layered conductors placed in a strong magnetic field **B** is studied theoretically in a wide range of the wave frequencies and at low temperature, when charge carriers are scattered mainly by impurity centers. By means of the Kubo method we have derived the surface impedance of a layered conductor under the condition when the separation $\hbar\omega_c$ between energy levels of electrons is much less than their chemical potential μ. The quasi-two-dimensional nature of the electron energy spectrum of layered conductors results in peculiar oscillatory dependence of the impedance on the inverse value of the magnetic field. The form of beats is typical for the oscillations arising from the quantization of orbital motion of charge carriers that possess the Q2D dispersion law. These oscillations are formed by the interference of the harmonics with the frequencies determined by the extreme-areas cross sections of the Fermi surface. Along with the beatings the low-frequency oscillations occur in layered conductors, their amplitude is small but decays weakly with temperature because the temperature smearing of the Fermi distribution function does not lead to a decrease in the amplitude of the oscillations. The shift of the the low-frequency oscillations phase is analyzed. The low-frequency fraction of the quantum oscillations may be observed at temperatures where the basic harmonics are utterly small.

New concept of statistical ensembles

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An extension of the standard concept of the statistical ensembles is suggested. Namely, a class of statistical ensembles with extensive quantities fluctuating according to an externally given distribution is introduced. Several examples in high energy physics are discussed. The proposed approach opens a room for new applications.

The penetration of high energy charged particles through bent crystals

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The review of mechanisms of high-energy charged particles deflection by bent crystals are proposed. The mechanisms which are connected with the plane channelling of particles in bent crystal planes and with particles reflection from bent crystal planes are considered. The special attention is paid to the stochastic mechanism of beams deflection which is connected with multiple scattering of particles on bent crystal atomic strings. Last CERN experiment [1] on discovery of stochastic mechanism of beam deflection and proposals of CERN and FERMILAB on following investigations of this effect are discussed.

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Quantum critical point, reentrant phase transitions and weak-universal critical behaviour of the spin-1/2 Ising-Heisenberg model with the pair XXZ Heisenberg interaction and the quartic Ising interaction

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The spin-1/2 Ising-Heisenberg model is defined on a two-dimensional lattice of edge-sharing octahedrons, each of them having four Ising spins in a basal plane and two Heisenberg spins in apical positions of the elementary octahedron. The ensemble of all Ising spins then forms a square lattice, which has a couple of the Heisenberg spins above and below a center of each elementary square face formed by four Ising spins. Assuming the pair XXZ Heisenberg interaction between two apical spins and the quartic Ising interaction between two apical spins and two basal spins from opposite corners of a square face of the same octahedron, the model under investigation becomes exactly solvable by applying the generalized star-square transformation that establishes a precise mapping relationship with the corresponding eight-vertex model on a square lattice generally satisfying Baxter's zero-field (symmetric) condition [1].

It is shown that the spin-1/2 Ising-Heisenberg model with the ferromagnetic pair interaction exhibits a remarkable phase diagram with two marked wings of critical lines, which merge together at a very special quantum critical point. As could be expected from the exact mapping to the zero-field eight-vertex model, the critical exponents vary continuously along the critical lines when changing parameters of the Hamiltonian. The changes of critical exponents are in accordance with Suzuki's weak universality hypothesis [2] in spite of a peculiar singular behaviour to emerge at a quantum critical point of the infinite order, which occurs at the isotropic limit of the XXZ Heisenberg pair interaction. The origin of observed reentrant phase transitions is explained from the disorder solution, as well as, the different ground-state degeneracies of two phases coexisting at the quantum critical point.

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On some effects in the ultraslow light phenomenon in Bose-Einstein condensates of alkali-metal atoms

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We propose a microscopic approach for a description of processes of interaction of the ideal gas of alkali-metal atoms with a weak electromagnetic radiation. The description is constructed in the framework of the Green-function formalism that is based on a new formulation of the second quantization method in case of the presence of bound states of particles (atoms). For a gas with the Bose-Einstein condensate (BEC) the dependencies of the propagation velocity and damping rate on the microscopic characteristics of the system are studied [1].

On the basis of the proposed approach the influence of the external homogeneous and static magnetic field on the slowing of electromagnetic waves in the condensate is studied. It is shown that the velocity of the pulses can be effectively controlled by the bias field [2].

The approach is generalized on the case on nonzero temperatures. We analyze the influence of the temperature effects on the slowing and absorption parameters of a BEC. It is shown that in the present experimental conditions the group velocity of pulses practically do not depend on the temperature in the region from the absolute zero to the critical temperature. We find the cases when the temperature effects in a BEC can play a significant role.

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Microscopic factors that control β-sheet registry in Amyloid fibrils formed by 11-25 fragment of Amyloid β peptide: Insights from computer simulations

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Short fragments of amyloidogenic proteins are widely used in studies of amyloid formation as convenient model systems. A recent solid-state NMR study of Tycko et al. [*J. Mol. Biol. 335 (2004) 247*] demonstrated that the fragment consisting of residues 11 to 25 of the amyloid β peptide involved in Alzheimers disease (Aβ11-25) can form fibrils composed of anti-parallel β-sheets. Interestingly, fibrils grown under neutral and acidic conditions were seen to possess different registries of their inter-β-strand hydrogen bonds. In an effort to explain the microscopic origin of this pH dependence, we study Aβ11-25 fibrils using methods of theoretical modeling. Several structural models are built for fibrils at low and neutral pH levels and examined in short molecular dynamics simulations in explicit water. The models that display lowest free energy, as estimated using an implicit solvent model, are selected as representative of the true fibrillar structure. It is shown that the registry of these models agrees well with the experimental results. At the neutral pH, the main contribution to the free energy difference between the two registries comes from the electrostatic interactions. The charge group of the carboxy terminal makes a large contribution to these interactions and thus appears to play a critical role in determining the registry.

Effective Hamiltonian for fluid membranes in the presence of long-ranged forces

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If the constituent particles of fluid phases interact via long-ranged van der Waals forces, the effective Hamiltonian for *interfaces* between such fluid phases contains – in lateral Fourier space – non-analytic terms $\sim q^4 \ln q$. Similar non-analytic terms characterize the effective Hamiltonian for two interacting interfaces which can emerge between the three possible coexisting fluid phases in binary liquid mixtures. This is in contrast with the structure of the phenomenological Helfrich Hamiltonian for membranes which does not contain such non-analytic terms. We show that under favorable conditions for the bulk densities characterizing a binary liquid mixture and for the long-ranged interparticle interactions the corresponding effective Hamiltonian for a model fluid *membrane* does not exhibit such non-analytic contributions. We discuss the properties of the resulting effective Hamiltonian, with a particular emphasis on the influence of the long range of the interactions on the coefficient of the bending rigidity.

Thermodynamic theory of stick-slip mode of ultrathin lubricant film melting

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The theory of ultrathin lubricant film melting is proposed in [1]. Within the framework of this theory the fluctuations are taken into account [2]. It is shown that fluctuations lead to the appearance of stick-slip mode of friction that is observed experimentally [3]. However, this mode has stochastic character and random transitions are realized between liquid-like structure of lubricant that corresponds to the non-zero shear stress, and solid-like structure at zero stress. Besides described above, the mode is observed in experiments in which these transitions have periodic character [3]. The purpose of this work is to describe such mode.

Within the framework of adiabatic approximation according to that the relaxation time of lubricant temperature is much shorter that its value for stress and strain, the two-parameter system is obtained, that is reduced to the unique differential equation of the second order. The system parameters are defined at which the damping oscillations occur during the relaxation process. Thus the special point of focus type is realized at non-zero value of stress. This situation corresponds to the periodic stick-slip mode of friction. However, the described mode is transitional, and liquid friction, corresponding to the sliding with constant velocity, is set in course of time. Taking into account the fluctuations it is shown in indicated case that the periodic stick-slip mode of friction is saved in time, since the action of fluctuations constantly leads the configurative point on phase plane on a nearby phase trajectory. Thus casual addition appears in the periodic mode that changes static and kinetic friction force in time. Since the dependence is not strictly periodic such mode corresponds to the experiments with chain molecules which are complex to form well-organized structures, due to that the fluctuations are laid on oscillations [3].

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Dynamics of the condensed Bose gas at the nonzero temperatures

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Bose-Einstein condensation (BEC) - one of the most interesting phenomena foreseen by quantum statistical mechanics. It is unique, because to be the exclusively quantum-statistical phase transmission and may occur without interaction between atoms. In the 1995 was got BEC "in a clean kind" in the trapped dilute ultracold clouds of alkaline metals.

Creation of the microscopic theory that described dynamics condensed Bose gas is very important problem. The foundation of theoretical description such quantum degenerate systems with spontaneous broken symmetry were laid by Bogolyubov in the paper about weakly-nonideal Bose gas. A central place in his theory occupies idea about separation of the condensate. To difference from Bogolyubov's model of weakly-nonideal Bose gas, the atomic Bose condensate is spatial inhomogeneous. At the temperatures close to zero (0 — $0.2\,T_{BEC}$), when almost all atoms being in condensate, the dynamics of atomic Bose condensate is describing by nonlinear equation for condensate wave function — Gross-Pitaevskii (GP) equation. In this temperature region GP equation very precise describe the experimental date with condensate (condensate oscillation, interferences of condensates etc). At higher temperatures, when an appreciable fraction of atoms is excited out of the condensate, the dynamics of the trapped gas becomes much more complicated since it now involves the coupled motion of the condensate and the non-condensate degrees of freedom. Thus description of the atomic Bose condensate at the nonzero temperatures in terms of GP equation is inadequate.

In this paper, from the first principles, we obtain generalized GP equation, which include the non-condensate degrees of freedom. This equation isn't closed, because dynamics of the non-condensate atoms is indefinite. For description of the non-condensate atoms, using Zubarev's method of nonequilibrium statistical operator, we derived Boltzmann quantum kinetic equation. Therefore we obtain complete dynamics of the condensed Bose gas at the nonzero temperatures.

Modified Bogolyubov's derivation of the two-fluid hydrodynamic equations for superfluid helium

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The two-fluid hydrodynamic equations for the superfluid 4He in the phenomenological consideration were constructed by Landau in 1941 [1]. At the microscopic level these equations were derived by Bogolyubov in 1963 [2]. Starting point in this paper is a set of equation of motion for local quantities (particle density, momentum density and energy density), which easy follows from Heisenberg equations for both creation and annihilation operators; as well as the equation for anomalous average $\langle\psi\rangle$. Thus, from the last follows a hydrodynamic equation for superfluid velocity.

For transition from formal equations of motion to hydrodynamic equations consider such stage of evolution of the system when it is approximate to equilibrium. Then it is possible to assume that in system is established the local equilibrium. At close to the thermodynamic equilibrium these parameters are slowly changed in space and time, therefore their gradients are small. Procedure of expansion by the gradients is formulated by introduction in equations of motion of the so-called parameter of homogeneity. Then an expansion by the gradients coincides with expansion by the "parameter homogeneities". Introduction of this parameter is carried out a formally way.

Our paper imitates the Bogolyubov's article [2], but we work with equations of motion for the correlation functions which are written in the mixed Wigner representation. It allows the expansion by the gradients directly realize, very easy and with the rigorous mathematic. In this paper we also developed method for calculation of the hydrodynamic flows. This formalism may be used for microscopic derivation two-fluid hydrodynamics of the superconductor and superfluid helium with pair condensate. This work was supported by SFFR of Ukraine (project No. F25.2/011).

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Two-dimensional electron gas in magnetic field

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The probability density current in states of charged particle in magnetic field is always not identically equal to zero because the vector potential of magnetic field cannot be equal gradient of wave function phase. A necessary condition for wave function of stationary states is closure of all streamlines in the area under investigation. Then axially symmetrical two-dimensional system is a simplest one for consideration. Thus, eigenfunctions are not localized in the vicinity of classical orbits as coordinates of orbit center do not commutate. The magnetic moment of eigenstate consists of an addend proportional to the orbital moment and an addend, which is always negative. An average magnetic moment of electronic gas cannot be equal to zero, as it is equal to a sum of products of magnetic moments of states and occupation numbers of these states. The derivative of the thermodynamic potential with respect to magnetic field does not coincide with this expression. The reason is that occupation numbers are proportional to degeneracy multiplicities of energy eigenvalues, which depend on magnetic field. The method is proposed which enables one take into consideration an angular momentum conservation law when deriving the probability density. Thus, this density depends on the effective Hamiltonian describing quasi-particles in the harmonic potential which intensity determines the magnetic field. Then degeneracy multiplicities do not depend on magnetic field and the paradox mentioned above is removed. The nonuniform electronic density and potential of the self-consistent field allowing for Coulomb interaction are determined by the density functional method. The energy spectrum of quasi-particles consists of two bands. The lower one, magnetic, is formed by the widened discrete levels, the conduction band is located above, and states in this one are similar to electronic states in the absence of magnetic field. The diamagnetic moment of gas is proportional to magnetic field, an area of circle and number of electrons. It is many times higher than Pauli paramagnetism. The diamagnetic current is disturbed over the area, therefore magnetization is nonuniform. Inhomogeneity of electrons density creates an electric field, which can be measured.

Raman scattering in the charge-density-wave phase of the spinless Falicov-Kimball model

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One of the simplest model with the strong electron correlation is the Falicov-Kimball model. The model possesses such quantum mechanical effects as metal-insulator transition, order-disorder phase transition and phase separation. Besides, the Falicov-Kimball model has exact solution within the dynamical mean-field theory (DMFT).

Raman scattering spectrum, including the nonresonant, mixed and resonant components, is determined for the charge-density-wave (CDW) phase of the spinless Falicov-Kimball model at half filling within DMFT. Its frequency dependence is investigated for different values of Couloumb repulsion (ranging from dirty metal to the Mott insulator) and for different temperatures. Obtained spectra reflect the structure of the many-particle density of states. The nonresonant response function is also determined for the case of the inelastic X-ray scattering (when both energy and momentum are transferred) [1]. In this case the most important features of spectra at low temperatures depend on the transferred momentum and an effective screening of uniform charge fluctuations, that is revealed by the careful examining of the first Brillouin zone. All investigations are performed for B_{1g}, B_{2g} and A_{1g} symmetries (which are usually examined in experiments).

Obtained results about the strong and weak temperature dependence of the low and high energy excitations, respectively, and the influence of the Couloumb potential on the shape of spectra give information about the charge dynamics in CDW-ordered phase which could be useful in experimental investigations of the corresponding compounds.

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Modeling of nanoindentation of α-graphite using registry-dependent interlayer potential

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Experimental investigations of the nanoscale friction between a tungsten tip of the friction force microscope (FFM) and graphite surface have revealed the existence of superlubricity in such a system. This phenomenon is manifested in a reduction of friction by orders of magnitude. Frictional force in the mentioned system exhibits strong dependence on the scanning direction of the FFM tip with the 60° symmetry of individual atomic layers in the graphite lattice. This fact and the agreement of the experiments with the numerical simulations carried out on the Tomlinson-based model have been the main reasons to argue that the superlubricity took place between the graphite substrate and a graphite flake, attached to the tip. However, in the experiments, there is no firm evidence for the cleavage of the flake and, to our knowledge, the existing theoretical models of superlow friction of graphite are based on the assumption of the presence of a graphene flake.

Here, we offer molecular dynamics simulations which reproduce flake formation for α-graphite. The graphite sample consists of three graphene layers with AB stacking. The bottom layer is static, covalent bonds between atoms in the remaining two dynamic layers are described via Brenner potential. For interlayer interactions registry-dependent potential with local normals by Kolmogorov is used. It is designed in such a manner that long-ranged van der Waals as well as short-ranged orbital overlap contributions to the cohesion in layered graphitic structures are taken into account. The sample is indented with adhesive absolutely rigid pyramidal tip and the heat is dissipated via Berendsen thermostat applied to all dynamic atoms. The influence of the value of interactions between carbon and tip atoms, the distance between atoms in the tip and the rate of indentation on the behaviour of the system are examined. The obtained force-versus-distance curves resemble experimental ones with jump-to-contact during loading phase and hysteresis during unloading. It is shown that flake formation takes place for higher values of carbon-tip interactions and indentation rates.

Equation of state for interior of giant planets

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We have calculated internal energy, free energy, entropy and pressure of a mixture of the metal hydrogen and atomic helium as the functions of the density and temperature. It is supposed, that the hydrogen presents itself the mixture of protons and electrons. Explored interval of pressures and density corresponds the conditions on the most planets of a solar system – Jupiter and Saturn. The perturbations theory series on degrees of an electron-proton and electron-atom interaction is used for calculation of thermodynamic potentials of mixture of metallic hydrogen and neutral helium. The electron subsystem was considered in the random phase approximation with taken into account the exchange interaction and the correlations in the local field approximation. A proton-proton, proton-atom and atom-atom interactions is taken into account in the hard sphere approximation. For determination of the hard sphere diameter the effective pair proton-proton and atom-atom interactions was used. For numerical calculations was taken into account the zero and second members of the series of a perturbations theory. It is analyzed an applicability of polytropic sphere model for modeling of the interior of Jupiter and Saturn and is offered value of a polytropic index. Founded density, pressure and the temperature on Jupiter as a function of distance from its centre. Evaluated possible hydrogen share in a composition of Jupiter and Saturn.

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2D non-Heisenberg ferromagnetic with complex exchange interactions

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We investigated the 2D magnetic system with anisotropic exchange interactions, which limiting cases are the 2D XY-model with biquadratic exchange interaction and the isotropic 2D non-Heisenberg ferromagnetic. The Hamiltonian of such a ferromagnetic system is given by

$$\mathcal{H} = -\tfrac{1}{2}\sum_{n,\acute{n}} J_{n,\acute{n}}(S_n^x S_{\acute{n}}^x + S_n^y S_{\acute{n}}^y + \Delta S_n^z S_{\acute{n}}^z) - \tfrac{1}{2}\sum_{n,\acute{n}} K_{n,\acute{n}}[\tfrac{\Delta}{3} O_{2n}^0 O_{2\acute{n}}^0 + \\ + O_{2n}^2 O_{2\acute{n}}^2 + O_{2n}^{xy} O_{2\acute{n}}^{xy} + \Delta(O_{2n}^{xz} O_{2\acute{n}}^{xz} + O_{2n}^{yz} O_{2\acute{n}}^{yz})] - \tfrac{1}{2}\sum_{n,\acute{n},i,j} V_{n\acute{n}}^{ij} S_n^i S_{\acute{n}}^j + \\ + \lambda\sum_n [u_{xx}(n) {S_n^x}^2 + u_{yy}(n) {S_n^y}^2 + u_{xy}(n) O_{2n}^{xy}] + \frac{E}{2(1-\sigma^2)}\sum_n [u_{xx}^2(n) + \\ + u_{yy}^2(n) + 2\sigma u_{xx}(n) u_{yy}(n) + (1-\sigma) u_{xy}^2(n)]. \tag{1}$$

Here we introduce the following notations: $J > 0, K > 0$ are the constants of the bilinear and the biquadratic exchange interactions, respectively; O_{2n}^p are the Stevens operators related with the spin operators as follows: $O_{2n}^0 = 3{S_n^z}^2 - S(S+1)$, $O_{2n}^2 = {S_n^x}^2 - {S_n^y}^2$, $O_{2n}^{ij} = S_n^i S_n^j + S_n^l S_n^i$; S_n^i is the ith component of the spin operator at the nth site; $u_{ij}(n)$ are the components of the elastic deformations tensor; λ is the constant of the magnetoelastic interaction; E is Young's modulus; σ is Poisson's ratio; $V_{n\acute{n}}^{ij}$ are the components of the magnetic dipole interaction tensor.

The results obtained show that the account of the exchange interactions anisotropy essentially changes the phase diagram of non-Heisenberg ferromagnetic. First of all, this is exhibited in the impossibility of the ferromagnetic ordering at $\Delta \longrightarrow 0$ (in this case the quadrupolar order is stabilized). The account of the magnetic dipole interaction leads to the realization of a spatially inhomogeneous QU-phase. Its inhomogenity is connected not with the spatial distribution of the magnetization, but with the change of the quadrupolar order parameters, which in their turn are related to the orientation of the main axes of the quadrupolar moments tensor. This result is predictive. As far as we know, an inhomogeneous quadrupolar phase has not yet been observed experimentally.

On the kinetic and hydrodynamic regimes of the Czirók-Vicsek model

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We consider the dynamics of the system of self propelling particles modelled via Czirók-Vicsek algorithm in continuum time limit. It is shown that the alignment process for the velocities can be subdivided into two regimes: "fast" kinetic and "slow" hydrodynamic ones. In fast kinetic regime the alignment of the particle velocity to the local neighborhood takes place with characteristic relaxation time. So that the bigger regions arise with the velocity alignment. These regions align their velocities thus giving rise to hydrodynamic regime of the dynamics. We propose the mean-field like approach in which we take into account the correlations between density and velocity. The comparison of the theoretical predictions with the numerical simulations is given. The relation between Vicsek model in the zero velocity limit and the Kuramoto model is discussed. Also we give simple estimation for the critical level of noise in the "mean-field" approximation for the vector and scalar types of noise.

DFT-based derivation of the microscopic model for the frustrated antiferromagnet Cs_2CuCl_4

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Recent experiments on the layered $S = 1/2$ frustrated antiferromagnetic compound Cs_2CuCl_4 indicate that in this material an exotic spin liquid (SL) state with fractional-spin quasiparticles might be realized. Even more fascinating is the fact that the analysis of the magnon dispersion spectrum in this system leads to the conclusion that Cs_2CuCl_4 can be described by a 2D triangular lattice of magnetic interactions. Whether the above mentioned SL state can exist in two dimensions is still a matter of debate among theoreticians. It is therefore clear that in order to develop a solid connection between theory and experiment an alternative determination of the microscopic model, such as by, e.g., the Density Functional Theory (DFT) method, for Cs_2CuCl_4 would be of great value.

In this presentation, we discuss the microscopic model for Cs_2CuCl_4 derived with the DFT approach. We also perform downfolding and tight-binding calculations and discuss the role of the electronic correlations in the compound. We find that inclusion of the on-site Coulomb interaction U for the Cu $3d$ electrons during the crystal structure relaxation is important in order to have agreement with the experimental observations.

Solvation forces in 2D Ising stripes

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The solvation forces for the 2D Ising stripes are calculated via exact diagonalization of the transfer matrix in two cases: the symmetrical case corresponds to identical boundary fields, and the antisymmetrical case to exactly opposite boundary fields. In the symmetric case the solvation force is always negative (attractive) while in the antisymmetric case the solvation force is positive (repulsive) at high temperatures and negative at low temperatures. It has a maximum close to the bulk critical temperature, changes sign close to the temperature of the wetting transition taking place in the semi-infinite system. The properties of the solvation forces are presented via the scaling functions describing their dependence on temperature, surface field, and stripe's width.

Ground states of anisotropic antiferromagnets with single ion and cubic anisotropy

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Anisotropic antiferromagnets in an external magnetic field show a rich variety of different phases meeting in phase transition lines and multicritical points. We study the dependence of the ground states of these systems in the three dimensional space on physical parameters as exchange, single ion and cubic anisotropy (see [1,2]).

One identifies four different ground states: the paramagnetic, the antiferromagnetic, the spin flop and the biconical ground state. In the case of absence of a cubic anisotropy the transition lines separating the different ground states can be calculated analytically, otherwise they have to be calculated numerically. We also considered the behavior of the staggered magnetization which characterizes the different ground states. From its behavior the order of the transition from one state to the other is determined.

The results obtained may be relevant for other systems since the antiferromagnetic model can be mapped to a lattice model where the biconical phase is interpreted as supersolid phase [3]. Recent renormalization group calculations show that such a phase would indicate the existence of a tetracritical point [4].

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Biconical critical dynamics

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Anisotropic Antiferromagnets in an external field (in three spatial dimensions) are fascinating systems showing several phases of magnetic ordering separated by lines of continous phase transitions meeting in a multicritical point. Renormalization group (RG) theory has recently shown that in general the biconical fixed point (related to a tetracritical point) is stable. Under special thermodynamic conditions the Heisenberg fixed point could be stable which then would lead to a bicritical point.

The dynamical critical behavior is especially rich. At the multicritical point two lines belonging to different universality classes meet. A new dynamical universality class (biconical dynamics) is governed by their meeting point (biconical fixed point). At low values of the external magnetic field the dynamics near the transition from the paramagnetic to the antiferromagnetic phase belongs to the universality class of model C (relaxational dynamics of the order parameter coupled statically to a conserved density). At higher values of the external magnetic field the transition from the paramagnetic to the spin flop phase belongs to model F (relaxational dynamics of the order parameter coupled statically and dynamically to a conserved density).

Our results [1] calculated within two loop order of RG theory bring about the presence of small static and even smaller dynamic slow transients. Therefore an effective critical behavior might be expected. The important advantage of this magnetic system is that the dynamical correlations of both the non conserved order parameter and the conserved density are in principle experimentally accessible by neutron scattering.

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Bogolyubov approach and Relaxed Optics

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Relaxed Optics is the chapter of modern physics, which is created for the explanation of the processes of the irreversible interaction light with matter [1]. This theory is based on the kinetic-energy classification of possible processes. For the classification of possible types phenomena the Bogolyubov chronological classification was complemented energy classification. This procedure may be represented may be represented as generalizing Sato theorem (theorem of reduction)from nonholonomic dynamical systems on kinetic phenomena.

This approach is more generalize as Bogolyubov approach. It allow to use various mathematical methods for thew modelling hierarchic dynamical processes. The using of BBGKI (Bogolyubov-Born-Green-Kirkwood-Ivon) chains for the explanation experimental data of irreversible interactions light and matter is very difficult. For the concrete realization of this classification for the modelling proper processes may be used methods of synergetic and catastrophe theory [2].

Another effective method of the realization of inhomogeneous time-energy hierarchy classification is the method of modelling hierarchy of saturation the excitation of proper chemical bonds. The proper chain of relaxation times is corresponded to step of saturation of excitation proper chemical bonds. This method allow to classify basic phenomena of interaction laser irradiation from Quantum Electronics (optical pump for laser irradiation) to Relaxed Optics (laser implantation) and synergetic (chaotization of laser irradiation).

The other possible applications of this method for the modelling mixing phenomena of Relaxed Optics are discussed too.

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Dynamic spin susceptibility and superconductivity in cuprates

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A relaxation-function theory for the dynamic spin susceptibility in the t–J model is presented. Spin correlation functions, staggered magnetization, uniform static susceptibility, and antiferromagnetic correlation length are calculated in a wide region of hole doping and temperatures. The self-energy is calculated in the mode-coupling approximation and the dynamical spin susceptibility is studied for various temperatures and hole doping. The obtained results are in a reasonable agreement with numerical simulations and experimental data. A relation of the obtained results to the spin-fluctuation theory of superconductivity in cuprates studied within the Hubbard model is briefly discussed.

Method of calculating the free energy of three-dimensional uniaxial magnet in an external field on the basis of the higher non-Gaussian distribution

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The microscopic approach to calculating the free energy of a three-dimensional Ising-like system in a homogeneous external field is developed in the higher non-Gaussian approximation (the ρ^6 model) at temperatures above the critical value of T_c (T_c is the phase-transition temperature in the absence of an external field). The free energy of the system is found by separating the contributions from the short- and long-wave spin-density oscillation modes taking into account the generalized point of exit of the system from the critical regime as a function of both the temperature and field variables. A calculation technique is based on the first principles of statistical physics and is naturally realized without any general assumptions and without any adjustable parameters. Our analytical calculations do not involve series expansions in the scaling variable and are valid near the critical point not only in the regions of the so-called weak and strong external fields but also in the crossover region between these fields, where power series in the scaling variable are not effective. The obtained expression for the free energy contains the leading terms and terms determining the temperature and field confluent corrections.

Density functional theory study of molecular oxygen interaction with the surface of stable binary nanoclusters of platinum and palladium

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Quantum-chemical calculations by means of DFT method showed peculiarities of electron density changes in the most active reaction sites for series of stable nanoclusters, such as $Pt_{37}X_{18}$ and $Pd_{37}X_{18}$ (where X – Cr, Fe, Co, Ni). Geometry structure as well as electronic characteristics for nanoclusters were calculated by means of self-consistent DFT method in generalized gradient approximation GGA with exchange correlation functional B88-LYP and the basis set double-zeta in valence approximation DZVP in frames of the program StoBe2007 [1].

We estimated details of molecular and atomic oxygen interaction with the surface of the most active binary nanoclusters $Pt_{37}Co_{18}$ and $Pd_{37}Fe_{18}$, situated over a monolayer substrate of graphite C_{82}. The main mechanism was proposed for this interaction. Chemical and electrochemical processes were distinctly divided, including molecular oxygen chemisorption, electron transition towards the chemisorbed molecule, dissociation of the surface oxygen molecular anion into its atom and singly charged ion and eventually reduction of the ion to the doubly charged specimen. The adsorption heat and activation energy of this stages were calculated on surface (111) for nanoclusters.

The sequence of the reactions possesses the lowest activation energies and the highest adsorption heats in three-folded sites. Therefore full reaction rate of oxygen reduction becomes extremely high.

It was shown that besides the nature of binary nanoclusters the structure of adsorptional and reaction sites is especially important. In particular, three fold position should be formed by 3 surface atoms of noble metals (Pt and Pd) with one atom of second component (Co and Fe) in the first sublayer. These nanoclusters would be proposed as effective materials for cathodes of modern low temperature fuel cells.

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A simple approach to ferroelectric ferromagnets: the case of $BiMnO_3$

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We discuss a simple phenomenological Landau theory of phase transitions with two coupled single-component order parameters and compare the results with available experimental data. They correspond to the case of a ferroic system, in which ferromagnetic and ferroelectric transitions originally occur at temperatures T_M and T_f, respectively. For $T_f > T_M$ the magnetoelectric coupling strongly renormalizes the magnetic transition temperature, $T_M \to T_{RM}$, as well as generates an additional anomaly in ferroelectric subsystem at the ferromagnetic phase transition temperature T_{RM}. Full susceptibility tensor has also been determined. The concept of Arrot plot is generalized to the situation when both types of order coexist. The results are in good overall agreement with experimental data for the ferroelectromagnetic $BiMnO_3$. We also estimate the contribution of Gaussian fluctuations of both order parameters, that lead to corrections to the mean-field specific heat. Those corrections are still insufficient even though other quantities agree quite well with experiment.

Superconductivity in an almost localized Fermi liquid of quasiparticles with spin-dependent masses and effective field induced by electron correlations

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We consider first the Cooper-pair bound state and the condensed phase of an almost localized Fermi liquid (ALFL) composed of quasiparticles in a narrow-band with the spin-dependent masses (SDM) and an effective field, both induced by strong electronic correlations. Both of these novel characteristics are calculated in a self-consistent manner for each of the phases separately. We analyze the bound states as a function of Cooper-pair momentum $|\mathbf{Q}|$ in applied magnetic field in the strongly Pauli limiting case (i.e. when the orbital effects of applied magnetic field are disregarded). The spin-direction dependence of the effective mass makes the quasiparticles comprising Cooper pair *distinguishable in the quantum mechanical sense*, while the condensed gas of pairs may still be regarded as composed of identical entities. The *Fulde-Ferrell-Larkin-Ovchinnikov* (FFLO) condensed state of moving pairs is by far more robust in the applied field for the case with spin-dependent masses than in the situation with equal masses of quasiparticles. Relative stability of the *Bardeen-Cooper-Schrieffer* (BCS) vs. FFLO phase is analyzed in detail on temperature - applied field plane. We conclude that the spin-dependent masses may play an important role in stabilizing high-field low-temperature (HFLT) unconventional superconducting states (FFLO being an instance) in systems such as $CeCoIn_5$, organic metals and possibly others.

Scaling of the renormalized single-particle wave function near Mott-Hubbard localization

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We discuss quantum critical scaling of the single-particle (Wannier) function near the Mott-Hubbard localization. This wave function is calculated in the Gultzwiller correlated state for the cubic lattices within a novel method previously applied to correlated nanoscopic systems. The wave function size and its maximum, as well as the system electronic energy, all scale as R^n, with $n \propto 1$, signaling the dominant role of the Coulomb interactions. We also relate the critical lattice parameter $R = R_c$ at the transition to the original *Mott criterion*. The results for 3-dimensional lattices are compared with exact results for the Hubbard chain.

Escape problem for fraction Brownian motion

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We consider a particle escape problem from a truncated harmonic potential well due to the presence of fractional Gaussian noise in the system. Our main aim is to calculate the mean escape time and the escape time probability density function, paying attention to the dependencies of these functions on the external noise intensity and its Hurst index.

We study persistent and antipersistent cases of fractional Gaussian noise marking both similarities and strong differences between them and unfold a set of unexpected peculiarities of fractional Brownian motion in the potential well alongside with its intuitively predictable ones.

Critical phenomena in systems with a joint multicritical and Lifshitz point

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We propose the model that allows one to describe the critical phenomena in systems which have a joint multicritical and Lifshitz-point-like behavior. The effective Hamiltonian for such type of systems includes arbitrary nonlinearities and higher gradients of the order parameters. An expression for the upper critical dimension (CD) of such systems is found from the convergence condition of renormalization procedure. We show that the considered model is invariant under the anisotropic scale transformations if the dimension of space is coincide with critical one. The infinitesimal operator of the corresponding Lie group is found. The analytical properties of the corresponding variation equations are discussed.

Catalytic CO oxidation reaction: lattice models and kinetic description

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The study of heterogeneous catalytic reactions have developed into a very active field of research in recent years. From the physical point of view, the kinetics of these reactions are of interest due to their richness and complexity related to such factors as surface heterogeneity, adsorbate-adsorbate lateral interactions, spontaneous and adsorbate-induced surface restructuring, and manifested in such phenomena as chemical waves, kinetic oscillations, and chaos.

Among the most studied reactions is the catalytic oxidation of carbon monoxide on platinum surfaces. Generally, catalytic CO oxidation reaction has been proven to proceed on Pt via a Langmuir-Hinshelwood mechanism in which both reactants are initially adsorbed on the surface. The goal of this work is to study catalytic CO oxidation on a Pt surface in the framework of a kinetic and a lattice-gas reaction models. On the basis of kinetic model we have found the stationary points of the system and analyzed them by their eigenvalues to reveal their stability. As it was found, at intermediate pressures the system exhibits two stable steady states, namely, a state of low reactivity with a predominantly CO covered surface, and a state of high reactivity with a largely oxygen-covered surface. The condition of the existence of the bistable region is analytically found and the bifurcation diagram is constructed. The effect of inactive impurities on the kinetics of catalytic reaction is studied. To give a more precise definition for model parameters, the ground-state phase diagrams of corresponding lattice models are investigated at temperature $T = 0$ by incorporating the nearest-neighbour interactions on a catalyst surface. The conditions of existence of nonuniform phases dependent on the interaction parameters are established and main types of ground-state phase diagrams are obtained.

On derivation of quantum kinetic equations and nonlinear Schrödinger equation

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We develop a new approach to the problem of the rigorous derivation of quantum kinetic equations from underlying many-particle dynamics.

At first we construct a solution of the Cauchy problem of the Bogolyubov chain of equations (BBGKY hierarchy) for marginal density operators of quantum many-particle systems in the space of sequences of trace class operators. Then we discuss the relationships between infinite-particle dynamics and quantum kinetic equations. A conventional approach to the problem of the rigorous derivation of kinetic equations from microscopic equations of the von Neumann or the corresponding quantum BBGKY hierarchy consists of the construction of a suitable scaling limit of the solution of the BBGKY hierarchy of equations with initial data satisfying the chaos property. As a result of the scaling limit a solution preserves the chaos property if the limit one-particle density operator satisfies the corresponding kinetic equation.

Our main result consists of the proof that, if initial data are completely defined only by the trace class one-particle density operator, the Cauchy problem of the BBGKY hierarchy is equal to the corresponding initial value problem of certain generalized quantum kinetic equation and an infinite sequence of explicitly defined functionals of a solution of the generalized kinetic equation. For initial data from the space of trace class operators we prove the existence theorem for the generalized kinetic equation.

The specific quantum kinetic equations such as the quantum Boltzmann equation and other ones, can be derived from constructed generalized quantum kinetic equation in the appropriate scaling limits. As a consequence of this result we derive the nonlinear Schrödinger equation for the Bose gas in the mean field limit. In conclusion we also discuss the problem of the derivation of quantum kinetic equations in the condensate state.

Phase diagram of length polydisperse Yukawa chain fluid

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An extension of the dimer version of Wertheim's thermodynamic perturbation theory is proposed and used to treat polydisperse mixture of the hard-sphere Yukawa chain fluid with chain length polydispersity. The structure and thermodynamic properties of the reference system, represented by the multi-component mixture of the Yukawa hard-sphere dimers, is described using polymer mean spherical approximation. Explicit analytical expressions for the Helmholtz free energy, chemical potential and pressure in terms of the two chain length distribution function moments are derived. The theory is used to calculate the full liquid-gas phase diagram, including critical binodal, cloud and shadow curves and distribution functions of the coexisting phases. Effects of fractionation in terms of the distribution function and its first and second moments are studied. Theoretical results of the theory at hand and employed recently high temperature approximation are in qualitative agreement with corresponding experimental predictions for the polydisperse mixture of the polymers in a single solvent. In particular both theory and experiment predict that longer chain polymers equilibrate to the liquid phase and shorter chain polymers are predominantly encountered in the gas phase.

Network harness: bundles of routes in public transport networks

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Public transport routes sharing the same grid of streets and tracks are often found to proceed in parallel along shorter or longer sequences of stations. Similar phenomena are observed in other networks built with space consuming links such as cables, pipes, neurons, etc. In the case of PTNs this behavior may be easily worked out on the basis of sequences of stations serviced by each route. To quantify this behavior we use the recently introduced notion of network harness [1,2]. It is described by the harness distribution $P(r, s)$: the number of sequences of s consecutive stations that are serviced by r parallel routes. For certain PTNs that we have analysed we observe that the harness distribution may be described by power laws. These power laws observed indicate a certain level of organization and planning which may be driven by the need to minimize the costs of infrastructure and secondly by the fact that points of interest tend to be clustered in certain locations of a city. This effect may be seen as a result of the strong interdependence of the evolutions of both the city and its PTN.

To further investigate the significance of the empirical results we have studied one- and two-dimensional models of randomly placed routes modeled by different types of walks. While in one dimension an analytic treatment was successful, the two dimensional case was studied by extensive simulations showing that the empirical results for real PTNs deviate significantly from those expected for randomly placed routes.

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Estimation of the critical points and the thermal scaling exponents for the square-lattice Ising antiferromagnet in nonzero uniform magnetic fields using its specific heat

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The specific heat for the square-lattice Ising antiferromagnet in a uniform magnetic field H is obtained from its exact grand partition functions on $L \times L$ lattices ($L = 4 \sim 16$), in an arbitrary nonzero external field at arbitrary temperature. In the limit $L \to \infty$, the antiferromagnetic (Néel) critical points for $H \neq 0$ are estimated from the locations of the specific-heat peaks. For the first time, the thermal scaling exponents y_t of the square-lattice Ising antiferromagnet in a magnetic field are obtained to be $y_t(H \neq 0) = 1.0$ directly from its specific heat, implying that the specific heat retains the logarithmic singularity at the Néel critical points even in a uniform magnetic field.

Instability of the nematic liquid crystal filled with sphere-like magnetic-impurity particles against formation of the modulated structures

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In the last decade, much attention has been attracted to Filled Liquid Crystals – highly disperse suspension of impurity particles in nematic liquid carrier. The tested objects are filled nematic liquid crystals-highly-disperse suspension of impurity particles within the nematic liquid carrier. The spatial distribution of rigid-sphere-like magnetic-impurity particles (with radii of 5 μm) within the host nematic liquid crystal is studied. Both the indirect effective interaction between the impurity particles by means of nematic medium and the direct magnetic interaction are considered as being responsible for the formation of (modulated) structures. In the general case, total interaction between the impurity particles includes several contributions-direct Van der Waals-type interaction (at short distances between the particles) and magnetic one as well as indirect interactions (through both the director-field distortions and the density inhomogeneities). The last one depends on temperature, density of nematic host medium and impurities' concentration. Such effective interaction controls the structure formation and properties of a system. Using continuum-mechanics and statistical-thermodynamics approaches, we analyze the necessary thermodynamic conditions for formation of modulated lamellar structures. This condition allows to calculate temperature of homogeneous-distribution stability loss and to estimate period of formed structures. The offered theoretical approach can be used to forecasting other anisotropic and inhomogeneous mesomorphic systems, which can find application by development of integrated-optics facilities to govern the light-beam passing (diffraction gratings of an optical range *etc.*).

Anharmonicity effects in the phonon spectrum of crystals with hexagonal close-packed lattice

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Expressions for the renormalized force constants of a crystal due to the effects of anharmonicity have been obtained in the self-consistent harmonic approximation.

The matrix of force constants have been calculated with taking into account contributions both central and non-central forces of interaction between atoms. The central forces of interaction have been described by Lennard-Jones potentials.

The calculation of phonon spectrum for symmetric directions of wave vector in the Brillouin zone for metals with hexagonal close-packed lattice have been performed.

The effects of anharmonicity and the contributions of non-central forces of interaction between the atoms of crystalline lattice in vibrational spectrum of hcp-Ti have been researched.

The frequencies of atomic vibrations of crystalline lattice and potential barriers for diffusion activation were found to diminish due to the effects of anharmonicity.

It was shown that with decreasing of ratio between the periods of crystalline lattice of c/a ($c/a < 1,633$) the anisotropy of dependence of frequencies of vibrations from a wave vector is increasing.

Translational and rotational dynamics of methanol molecules in $NiCl_2$–methanol solutions: MD simulations vs. quasi-elastic neutron scattering

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The high-resolution quasi-elastic neutron scattering (QENS) technique has been applied to study the translational and rotational diffusion of methanol molecules in pure methanol (MeOH) at different temperatures and various $NiCl_2$ concentrations. Molecular dynamics (MD) simulations have been carried out in the NVT ensemble to explore the particle dynamics and microscopic structures of the experimentally investigated systems.

The translational diffusion coefficients derived from the QENS measurements of pure MeOH at the different temperatures agree well with the values reported in literature. Our results clearly indicate that the translational diffusion coefficient of methanol decreases (*i*) with decrease in temperature, and (*ii*) with increase in the concentration of $NiCl_2$ in MeOH, whereas the rotational diffusion coefficient is not so affected by variation of temperature or electrolyte concentration. The present MD simulations confirm the above experimental findings.

The MD results show that mainly the solvent molecules present in the bulk govern the dynamic behaviour of MeOH molecules in its electrolyte solutions. The translational diffusion coefficients of the Ni^{2+}, of MeOH molecules in the first solvation shell of Ni^{2+}, and also of its counter-ion, the Cl^-, are very close to each other and follow similar trends with change in concentration of the electrolyte.

Analysis of molecule dynamics in terms of diffusion coefficients and autocorrelation functions of angular and centre-of-mass velocities, and unit vectors of dipole moment show that a cation of small size and high charge, such as Ni^{2+}, forms dynamically well-defined solvation shell. Also, with decrease in the ion-molecule distance, the mobility of solvent molecules decreases significantly for such ions of high charge density.

Critical velocities and stationary waves in a two-component supersonic superfluid

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The properties of a two-component superfluid system are described by the three-velocity hydrodynamics. Since superfluid components can flow without friction, superfluid velocities of the components may differ from each other and from the velocity of the normal component. The question on critical velocities in the three-velocity hydrodynamics requires special consideration because in general case the spectrum of the excitations cannot be found from the Galilean transformation. One of the experimental methods to determine critical velocities for trapped ultracold gases consists in the observation of density excitations induced by some object moving through the condensate. Since the Bogolyubov spectrum has a dispersion a motion of an object through a superfluid system can lead to an occurrence of stationary waves.

Properties of stationary waves in a flow of a two-component quasi-two-dimensional Bose-Einstein condensate past an obstacle are studied here. It is shown that stationary waves arise when the Landau criterium is broken. It yields a joint condition on absolute values of the superfluid velocities of the components and on the angle between their directions. At the same time, the existence of stationary waves is restricted from above by the condition that relative velocity of the components does not exceed some critical value (otherwise a spatial separation of the components takes place). It is shown that several qualitatively different stationary wave patterns are possible. If the velocities are the same, (one) two sets of waves can appear when the velocities exceed the phase velocity of the lower (higher) hydrodynamic mode. If only one component moves then only one set of waves can emerge. If the velocities are equal in modulus and the angle between the velocities is close to $\pi/2$, two or tree sets of interfered stationary waves can arise. The two-dimensional images of the total density and relative density oscillations in the stationary wave pattern are obtained. It is established that in most cases the waves are visible in total density images as well as in relative density images, but the relative density images are more contrast.

The choice of the proper order parameter and the asymmetry effects in the critical behavior

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The effects of the critical behavior in real systems caused by the asymmetry of the Hamiltonian are discussed within the framework of the canonical formalism. It is shown that the spurious $\tau^{2\beta}$-term in the critical asymptotic behavior of the rectilinear diameter of the density:

$$\phi_d = D_{1-\alpha}\,|\tau|^{1-\alpha} + D_{2\beta}\,|\tau|^{2\beta} + \dots\,, \quad \tau = (T_c - T)/T_c$$

is caused by the asymmetrical terms of the Hamiltonian. Within the perturbation theory these are the quasilocal $\phi\,(\nabla\phi)^2$ and the local ϕ^5 terms. It is shown that the ratio of the amplitudes $D_{1-\alpha}/D_{2\beta}$ takes the universal character modulo non-universal factor which depends on the thermodynamic class of the corresponding states. This implies also the universality of the ratio of the amplitudes of these singular terms in isomorphic variables. They are conjugated (in thermodynamical sense) to the canonical order parameter field which restores the symmetry of the Hamiltonian. As a sequence, the equation of state in such variables is fully symmetrical with respect to coexisting phases. The procedure of calculation of these variables performed for the number of model equations of states for molecular liquids. This conclusion is checked via analysis of the experimental data for a number of liquids. The dependence of the critical amplitudes on the intermolecular interactions is discussed. The structure of the next to leading asymptotic terms in compressibility and the singularity of the Tolman length are determined. The connection between the proposed approach and the "complete" scaling hypothesis proposed by M. Fisher and coll. is discussed.

Brownian motion as a model of evolution of nonequilibrium system

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According to the principles of thermodynamics, any system being in contact with the thermal bath passes in the equilibrium state for the relaxation time. The paper presents a model of Brownian motion of the system which allows one to determine its stationary states far from the equilibrium. The stationary distribution function of a nonequilibrium state can be represented by none of the known equilibrium distributions. It is shown at which conditions the equilibrium states are realized, and new stationary states of nonequilibrium systems are predicted.

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On equilibrium charge distribution above dielectric surface

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The problem of the equilibrium state of the charged many-particle system above dielectric surface is formulated. We consider the case of the presence of the external attractive pressing field and the case of its absence. The equilibrium distributions of charges and the electric field, which is generated by these charges in the system in the case of ideally plane dielectric surface, are obtained. The solution of electrostatic equations of the system under consideration in case of small spatial heterogeneities caused by the dielectric surface, is also obtained. These spatial inhomogeneities can be caused as by the inhomogeneities of the surface, as by the inhomogeneous charge distribution on it. In particular, the case of the "wavy" spatially periodic surface is considered with the account of the possibility of the surface charges presence.

Polarization features of acoustic waves and Green functions in uniaxial nematic liquid crystals

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In the report the results of investigation of uniaxial nematic liquid crystals with rod-like and disc-like molecules are presented. The work is based on Hamiltonian approach which is characterized by establishment of the set of reduced description parameters, macroscopically full specifying investigated physical systems, Hamiltonian as the function of these parameters and obvious kind of Poisson brackets for the whole set of reduced description parameters. For the adequate description of nematic liquid crystals, besides densities of momentum, entropy and number of particles, additional dynamic parameters are introduced. They are the unit vector of spatial anisotropy (the director) and the conformational degree of freedom (rod length or disc diameter). On the basis of the approach, developed by as, the nonlinear dynamic equations taking into account molecules size and shape are derived. The acoustic spectra of collective excitations for investigated condensed matters are found out and it is shown, that taking into account molecules size and shape leads to the appearance of the second sound already in adiabatic approximation. The polarization features of acoustic waves in considered liquid crystals are investigated. It is clarified, that the first and second sounds are superposition of the longitudinal and transversal components. The nonlinear dynamic equations for the considered liquid crystals with regard to the anisotropy axis and conformational parameter in external alternating field are derived and the kind of sources in the dynamic equations corresponding to this field is determined. The analytic expressions for low-frequency asymptotics of Green functions are obtained. It is clarified, that in this case Bogolyubov theorem does not work, because orbital momentum is not the additive integral of motion and is not the part of the set of reduced description parameters.

Crystalline ordering of colloidal particles dispersed in liquid crystals

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We present a mean field theory to describe phase separations in mixtures of a liquid crystal and a colloidal particle. By taking into account a nematic and a smectic A ordering of liquid crystals and a crystalline ordering of colloidal particles, we calculate the phase diagrams on the temperature-concentration plane. We predict various phase separations, such as a smectic A-crystal phase separation and a smectic A-isotropic-crystal triple point, etc., depending on the interactions between a liquid crystal and a colloidal surface. Inside binodal curves, we find new unstable and metastable regions which are important in the phase ordering dynamics. We also find a crystalline ordering of colloidal particles dispersed in a smectic A phase and in a nematic phase. The cooperative phenomena between liquid crystalline ordering and crystalline ordering induce a variety of phase separations.

Nucleation and cavitation phenomena in a fluid of two-level atoms in the presence of external electromagnetic fields

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We consider a simple model of a fluid of two-level atoms in the presence of an external electromagnetic field. Moreover, we distinguish two particular cases: 1) the case of static electric field (which obviously modifies the interatomic interactions) and 2) the case of electromagnetic field with the frequency which corresponds to the excitation energy of the atom (resonance irradiation leads to appearance of excited atoms and, as a result, to appearance of new (resonance) interatomic interactions).

To examine nucleation and cavitation phenomena in the fluid we use the density functional approach [1]. More specific, we use the density functional of the grand-canonical thermodynamical potential, which takes into account the short-range interactions within the Carnahan-Starling approximation and the long-range interactions within the mean-field approximation [2]. We calculate the nucleation barrier for the vapor-to-liquid phase transition and the cavitation barrier for the liquid-to-vapor phase transition and discuss how these quantities change owing to the static electric field or because of the presence of excited atoms.

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Almost exact multiple time scale molecular dynamics

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The vast majority of systems in physics, chemistry, and biology are characterized by the coexistence of dynamical processes with different time scales. Molecular dynamics (MD) is a powerful tool which is widely used to study various phenomena in such systems. In view of the restricted capabilities of computers, the main factor responsible for further progress in MD modeling is the increase of efficiency of integrating schemes. A lot of multiple time stepping (MTS) techniques have been devised over the years to improve the efficacy of MD simulations. Despite the previous achievements, all the known MTS algorithms are precise only to the second order in the time steps. This means that only modest accuracy of the computations can be reached.

In the present investigation we propose a novel MTS method for the integration of motion in MD simulations of many-particle systems. It combines special phase-space transformations with a high-accuracy reversible factorization of the time evolution propagator into analytically solvable parts related to different time scales. This allows one to overcome principal limitations imposed on efficiency of the simulations in standard MTS algorithms. Comparison with the well-recognized previous MTS approaches has shown, in particular, that the new method is able to substantially increase the precision of the integration incurring nearly the same computational efforts. This makes the MD calculations almost exact already at typical sizes of the time steps.

Our method is quite general and can be applied to various areas including hybrid Monte Carlo and *ab initio* MD simulations. It can also be extended to more complicated non-Hamiltonian systems and statistical ensembles with additional degrees of freedom and arbitrary numbers of time scales.

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The electronic structure of the Abrikosov vortex core and the pinning on a cylindrical defect

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The model of the Abrikosov vortex pinning on a cylindrical defect is proposed. The pinning of the vortex core is modelled as the bound state of the couple of elementary excitations within the potential well formed by both the defect and the magnetic field which penetrates into the vortex core. It is shown that in the limit $\kappa \gg 1$ the potential for the vortex core excitations can be treated within the zero-range potential method. The corresponding pinning energy is represented as following:

$$E = E_0 + \alpha E_1 + o(\alpha)\,,$$

where $\alpha = \{\frac{\Phi}{\Phi_0}\}$ is the fractional part of the magnetic flux Φ through the vortex core and Φ_0 is the magnetic flux quantum. Here E_0 is the pinning energy contribution due to the defect and E_1 is the additional magnetic energy, which in general depends on E_0. Basing on the representation for the energy of pinning we use the variational method to estimate the characteristics of pinning: the energy, the force and the density of critical current. The comparison with the data for YBaCuO is made. The results obtained are in a good agreement with the known theoretical results.

Kinetics of current formation in nanomolecular devices

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Recent investigation of conductive properties of nanomolecular devices (nanoleads + organic molecule) shows a strongly specific behavior of their nonlinear current-voltage characteristics including a rectification and Coulomb blockade. It has been recently revealed that such a nonlinearity is generally dictated by a molecular recharge which appears during an electron/hole transmission through the molecule. Since the recharge is connected with real occupation of the molecule by extra electrons coming from the adjacent nanoleads, a formation of the current is completely controlled by kinetic processes within the device. Based on the nonequilibrium density matrix method and using the Bogolyubov's approach for decoupling of the many-particle distribution functions, a closed set of kinetic equations for the state occupancies of the device is derived along with respective charge transfer rates. Kinetic equations have been employed to analyze an evolution behavior of the current in nanomolecular device with a single frontier molecular orbital. It has been shown that just after a sudden alteration of an applied bias voltage, the giant switch-on and switch-off currents can be formed in the device if only a coupling of the molecule to the leads differ strongly from one another. Just this circumstance is responsible for a rectification effect in the device. Both a switch-on/off effect and a rectification effect are especially pronounced at a resonant regime of charge transmission through the molecule when the capture of transferred electrons by a molecule occurs with a high probability. It is important to underline that in a nanomolecular device, a charge hopping kinetic process controls the formation not only a nonelastic component of the current but a tunnel current component as well. If more then one extra electrons occupy a nanomolecule, then due to repulsion between the extra electrons a current through the nanomolecular device can be blocked (Coulomb blockade).

Thermodynamics of adsorption and properties of simple fluids on solid surfaces modified by layers of grafted chains. Recent advances from density functional approaches

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Recent experimental research in new materials, processes and devices involving fluids on chemically modified solid surfaces motivated us to extend theoretical modelling and versatility of density functional approaches and investigate this class of systems. Specifically, we are interested in phenomena occurring at liquid-solid interfaces under the conditions that a solid is covered by a layer of chain molecules (polymers) that are grafted by terminating segments. This setup provides the possibility to influence intentionally the properties of the interface as well as to observe some new surface phenomena. The principal issue of the theory is in appropriate modelling of the grand thermodynamic potential of the systems in question. The effects of connectivity of segments that form chains, all non-bonding interactions between fluid species and fluid-solid interactions are taken into account. An ample set of results published during last few years in the Journal of Chemical Physics and Journal of Physical Chemistry is reviewed in detail.

Classical and quantum anisotropic Heisenberg antiferromagnets

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We study classical and quantum Heisenberg antiferromagnets with exchange anisotropy of XXZ-type and crystal field single-ion terms of quadratic and cubic form. The magnets display a variety of phases, including the field-induced spin-flop (or, in the quantum case, spin-liquid) and biconical (corresponding, in the quantum lattice gas description, to supersolid) phases. Applying mainly ground-state considerations, MC and DMRG methods, the impact of quantum effects and lattice dimension is analysed. Interesting critical and multicritical behaviour may occur at quantum and thermal phase transitions.

Compact group approach to analysis of the dielectric and optical characteristics of finely dispersed systems and liquids

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A new method for studying the long-wavelength dielectric and optical characteristics of particulate systems, such as dielectric composites, suspensions, and liquids, is presented. The method is based upon the concept [1] of macroscopic compact groups of particles, according to which a particulate system is treated as a set of macroscopic regions that have typical scales much smaller than the wavelength of probing radiation, but yet include sufficiently large numbers of particles to reproduce the properties of the entire system. The analysis begins with consideration of the electrodynamic problem on propagation of an electromagnetic wave within such a system. The formal solutions for the electric field and induction are represented in the form of infinite iterative series. With a special representation for the electromagnetic field propagator, the short-range multiple reemission and correlation effects within compact groups are shown to be the primary factors responsible for the formation of the above characteristics of the system. Their averaged contributions can be singled out from all terms in the iterative series and then effectively summed up. Depending on the problem to be solved, either averaging over volumes much greater than the scales of compact groups or statistical averaging involving many-particle correlation functions can be applied.

The efficiency of the method is demonstrated by using it to calculate the effective dielectric constant of systems of hard dielectric particles, which are in general inhomogeneous and anisotropic in both shape and dielectric properties, and to incorporate short-range multiple scattering effects into the theory of light scattering by systems of hard spherical particles. The results obtained are discussed.

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Statistical theory of crystals phases: the bound of thermodynamic stability

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Phase transformations in the solid state represent an interesting physical problem. Besides, they can have important meaning for practical applications. Accurate estimates of the thermodynamic limits of different crystal phases as equilibrium structures can play the decisive role when selecting the materials as candidates for use in real devices. Recently, it was established experimentally [1] that the fcc phase of Xe undergoes a transition of martensitic type into some intermediate phase having the sings of the hcp modification. In the present communication it is shown that the equations of the statistical theory of crystals [2,3] admit the existence of the equilibrium space-periodic solutions typical for the fcc phase of the noble gas crystals only in some definite domain of pressures and temperatures. The boundary of these domain is a line at which the fundamental thermodynamic condition of the positivity of the isothermal compressibility of the system is broken. The theoretical estimate of the limiting pressure of the loss of the thermodynamic stability of the fcc phase under discussion leads for Xe at the room temperature to the value ≈ 1.5 GPa. This value is rather close to the pressure at which the above said martensitic transition is fixed in Xe [1]. It seems useful to extend the range of the experimental study of the polymorphic transitions in order to stimulate further theoretical investigations of the effect of the thermodynamic instability in crystals.

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The theory of electro-magnetic radiation of electron transiting through the resonance-tunnel structure

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The electro-magnetic radiation arises when the electrons are transiting through the resonance-tunnel nanostructure. This phenomenon is actively used for the creation quantum cascade lasers (QCL's) with unique physical characteristics. Besides, the radiation of QCL is in sub- millimeter range of wave lengths is actual for the applied utilization. The main problems are to produce a device working at the room temperature, has the minimal magnitude of the excited current and the maximal strength of electro-magnetic radiation in demanded range.

According to the practical urgency, it is necessary to develop the theory of electro-magnetic radiation arising when the electrons are transiting through the open nano-RTS with quasi-stationary states. The consequent theory correlating to the experimental data obtained for the QCL's, is still absent. The theoretical papers of this direction can be conditionally divided into two groups: in the first, it is used the Hamiltonian of the system, containing many fitting parameters, varying which one can obtain the correlation to the experiment; in the second, it is studied the model system within the approximation of effective masses and rectangular potentials for the electron in RTS. The disadvantage of the first approach is that the physical processes in RTS here are described unclearly. In the second one, the physical processes are clear but the rectangular potentials are changed into the delta-like ones, due to the mathematical obstacles, bringing to the rather rough evaluations which can not be compared to the experimental data. The consistent theory of electron-phonon interaction in RTS is absent at all.

In the paper it is established the theory of generalized conductivity in three-barrier nano-RTS. The system Hamiltonian contains the electron energy (with known effective masses and rectangular potentials) and the energy of electron interaction with electro-magnetic field. The spectral parameters (resonance energies and widths) of electron quasi-stationary states in RTS are calculated and analyzed. There are obtained the optimal sizes of RTS components, which can improve the physical characteristics of three-barrier lasers.

Stationary and quasistationary electron spectrum in quantum wire and quantum anti-dot with impurity

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Recently, the investigation of open or resonance-tunnel semiconductor heterostructures has been essentially accelerated. It is caused by the unique perspectives of their utilization for the creation of field transistors, diodes and quantum cascade lasers.

The theory of electron energy spectrum and wave functions in open spherical quantum dots has been developed using the S-matrix method within the effective masses and rectangular potentials approximations. It allows obtaining the dependences of electron energy spectrum and life times on the geometrical parameters. However, using it for the investigation of exciton spectrum or interaction between electron and impurity in open nanosystem is rather sophisticated or simply impossible. We propose the alternative method of electron energy spectrum investigation in open quantum dots at the base of two models:

1. For open semiconductor cylindrical quantum dot (CQD) embedded into the quantum wire, the one-well open CQD is approximated by the respective complicated closed three-well CQD with the very big heights of outer QD's. When the heights of outer QD's are varying till the physical infinity, the stationary electron spectrum is transforming into the quasi-stationary one with the respective resonance energies and widths. The proposed mechanism of three-well closed CQD (inside of QW) transformation into the single one-well open CQD (inside of QW) allows solving the problem of exciton spectra in open CQD (inside of QW).

2. The electron in the Coulomb field of donor impurity, placed into the center of spherical anti-dot is under study. Due to the presence of both Coulomb potential of impurity and rectangular potential of quantum anti-dot, the electron potential consists of two potential wells: inner-deep and outer-shallow. Consequently, the electron energy spectrum consists of stationary and quasi-stationary states. The energy spectrum and life times in the open nanosystem are obtained within the probability distribution of electron location in the inner well and barrier.

Dielectric, piezoelectric, elastic, dynamic, and thermal properties of KH_2PO_4 type ferroelectric compounds

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Within the framework of the modified proton ordering model for KH_2PO_4 family crystals that takes into account linear over strains ε_6 and ε_4 contributions to the proton subsystem energy and neglects tunneling, we use a four-particle cluster approximation to calculate the corresponding thermodynamic potentials of the system. Using appropriate equations of state, we find spontaneous polarization, longitudinal and transverse dielectric permittivities of mechanically free and clamped crystals, piezoelectric characteristics related to shear strains ε_6 and ε_4, elastic constants c_{66} and c_{44}, and specific heat of the crystals.

Dynamic characteristics of the crystals are explored within a stochastic Glauber approach for the proton subsystem with taking into account dynamics of piezoelectric strains ε_6 and ε_4 via Newtonian equations of motion. Ultrasound velocity and attenuation, longitudinal and transverse dynamic permittivities of mechanically free and clamped crystals of the KH_2PO_4 family crystals are found.

A thorough numerical analysis of the calculated characteristics is performed for the MD_2XO_4 (M = K, Rb, ND_4; X = P, As) compounds. The quantities for partially deuterated crystals are calculated in the mean crystal approximation. The obtained sets of the model parameters allow a proper description of available experimental data for these ferroelectrics. Phenomena of crystal clamping by a high-frequency field and piezoelectric resonance are described. Peculiarities of the ultrasound attenuation in these crystals are described. A presence of a cut-off frequency in the frequency curves of attenuation is predicted. It is shown that taking into account piezoelectric coupling hardly affects the calculated spontaneous polarization or specific heat, but gives rise to differences in dielectric permittivities of mechanically free and clamped crystals and increases the relaxation dispersion frequency.

Influence of transverse electric fields on physical properties of the Rochelle salt $NaKC_4H_4O_6 \cdot 4H_2O$

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A four-sublattice order-disorder model with taking into account piezoelectric interactions and external transverse electric fields is developed for description of phase transitions dielectric, piezoelectric, elastic and thermal properties of the Rochelle salt crystal. Our model is a generalization of four-sublattice model proposed in [1] and Mitsui model with taking into account the piezoelectric effects [2]. Within a mean field approximation specific heat, dielectric constants $\varepsilon_{11}^{\varepsilon}$, $\varepsilon_{22}^{\varepsilon}$, $\varepsilon_{33}^{\varepsilon}$ for a clamped crystal and $\varepsilon_{11}^{\sigma}$, $\varepsilon_{22}^{\sigma}$, $\varepsilon_{33}^{\sigma}$ for a free crystal, elastic constants c_{44}^{E}, c_{55}^{E}, c_{66}^{E} at constant field and c_{44}^{P}, c_{55}^{P}, c_{66}^{P} at constant polarization, piezoelectric moduli d_{14}, d_{25}, d_{36}, e_{14}, e_{25}, e_{36}, h_{14}, h_{25}, h_{36}, g_{14}, g_{25}, g_{36} under external transverse electric fields E_2 and E_3 are calculated. The set of the theory parameters providing the best fit to the available experimental data is found.

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Novel approaches in statistical physics

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In the given report the attention to use of a thermodynamic limit is paid at optimization problems research by methods of statistical physics [1]. In particular, in known minority game model [2,3] it is connected with treatment of parameter β/N, where β has a sense of inverse temperature, N is a number of dynamic variables (macroscopic). In papers [2,3] the given parameter is considered to be a small quantity and we expand in terms of it. That is how it is acted in problems of statistical physics. However, in an optimization problem where the limit β-infinity is considered only, such approach looks disputable. The given report presents the results of researches of an optimization problem in minority game model in gauss approach where expansion in terms of parameter β/N is not used directly. The point of the given approach is that at averaging over discrete variables in a replica method a transition to averaging over continuous variables with normal (gauss) distribution is carried out. As a result an effective Hamiltonian was received and the basic condition of system in space of dynamic variables was investigated. Calculations carried out in symmetric replica approach, and also with symmetry breaking replica. The received results are compared to the known approach from references.

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Electron density of states for doublewalled carbon nanotubes

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The method of zero-range potentials is used to investigate the one-electron density of states in double-walled carbon nanotubes. The results obtained were compared with those obtained as the sum of densities for the single-walled nanotube constituents, which were also calculated within the same method. The results for semiconductor tubes have proved to deviate in the Van-Hove's peak positions and widths by no more than 1% everywhere except for the band gap edges, where the differences can amount to as high as several percents. The intertube interaction leads to narrowing of the gaps in the both constituent tubes.

Photoinduced control of single molecule conductance

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Due to a potential application of single molecules as basic elements for a future electronics, the studies of conductive properties of organic molecules have attracted considerable interest. Molecular devices (single molecules embedded in between two metallic electrodes) are already fabricated with different functional properties like as a current rectification and a switching effect. Special interest has been focused on the role of external time-dependent fields controlling the conductance of single molecules. In particular, the use of electromagnetic radiation such as a laser light, can provide a convenient method to operate a single-molecule conductance.

To gain insight into investigation of a photoinduced single-molecule conductance, we propose a model where the photoinduced current is formed through a specific type of molecule (connecting two nanoelectrodes) which exists in its neutral, single-charged and photoexcited states. In this model, the conductance is governed by a specific charge-transfer processes. Respective kinetic equations are derived with use of nonequilibrium density matrix method. Exact solution of the closed set of kinetic equations is applied to analyze a time-dependent current formation. For a steady state regime, the analytical expression for a combine elastic and inelastic photoinduced inter-electrode current is derived. The influence of light frequency on current-voltage and conductance-voltage characteristics is analyzed in detail. The effect of photoinduced switching between the low and the high molecular conductance states is theoretically predicted. Additionally, in the case of asymmetric voltage drop across the molecule, a current rectification is observed.

Cold excitons in a quantum degenerate regime

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Collective quantum mechanical phenomena such as superfluidity and superconductivity are observed for particles at high density and low temperature. These collective effects can also take place in optically manipulated materials through a precise control of light-matter interactions. In particular, photo-generated electrons and holes in semiconductors provide a unique opportunity to examine macroscopic quantum phenomena such as the crossover from quantum degenerate bosonic ensembles (Bose-Einstein condensate states of excitons) to Fermi-degenerate electron-hole ensembles.

The 1s excitons of the yellow series in Cu_2O are the most promising candidate to demonstrate experimentally exciton BEC. Much effort has been devoted to this topic using 1s para-excitons, which have completely parallel electron-hole spin states and an extremely long lifetime. However, the dynamics of para-excitons is not well understood yet since there is no direct and sensitive method for their detection. We developed a time resolved mid-infrared pump and probe spectroscopy technique to detect excitons by measuring the absorption associated with internal excitonic transitions (1s to np) [1,2]. In combination with a phase space compression scheme [3] of pulsed two-photon excitation of ortho-excitons [4], we successfully generated super-cooled ortho excitons and observed excitonic Lyman series transitions from 1s to np ($n = 2, 3, 4, 5$) states [5]. We obtained information on the wavefunction of the lowest 1s exciton state which enables evaluation of density and temperature of para-excitons. We also developed CW laser-based excitonic Lyman spectroscopy to examine the para-exciton dynamics into a longer timescale and determined the lifetime and collision induced loss parameters in a steady state regime [6]. In this talk, novel aspects of collective quantum phenomena obtained from a series of experiments will be discussed, including recent work on para-exciton trapping in a strain potential and high density exciton generation using shaped pulse two-photon excitation [7].

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1D systems embedded into 3D space

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Real multi-particle systems like nanowires, nanotubes, polymer chains, which are modeled as one-dimensional, actually are embedded into the three-dimensional space. In this talk we discuss the effect of implicit three-dimensionality onto equilibrium characteristics and correlation functions of 1D systems.

Transverse field effect on thermodynamic properties of the spin-3/2 Blume-Capel model on rectangular lattice

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Influence of transverse field on the spin-3/2 Blume-Capel model is studied within the mean field approximation. Phase diagrams in the (transverse field, temperature) plane are constructed for different values of single-ion anisotropy. Temperature dependences of thermodynamical functions for different values of the model parameters are obtained.

It is shown that at some sets of the model parameters the re-entrant and double re-entrant phase transitions between the antiferromagnetic and the paramagnetic phases take place. The same behaviour is found out inside the antiferromagnetic phase.

Equilibrium states and dynamics of magnetics with spin 1

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The classification of equilibrium states of magnetic condensed media is carried out, which symmetry is spontaneously broken relatively to rotations in spin space and translations in configurational space. The cases of quadrupolar and vector order parameter are considered. Conditions of residual symmetry and spatial symmetry of equilibrium states for such media are formulated. In the case of vector order parameter the connection of these conditions with paramagnetic, ferromagnetic, antiferromagnetic, ferrimagnetic and spiral magnetic states is established. For magnetics with quadrupolar order parameter the connection of mentioned conditions with uniaxial and biaxial magnetic nematics, magnetic cholesterics and dual spiral magnetic is found out.

Dynamics of magnetics with spin 1 in the context of Hamilton's approach is considered. For such magnetic systems there are three different cases possible. In the first of them SU(3) symmetry of equilibrium state coincides with Hamiltonian symmetry, the spin and quadrupolar matrix are motion integrals. In the second case symmetry of equilibrium state is lower than SO(3) Hamiltonian symmetry. At that the quadrupolar matrix is order parameter and only spin vector components remain motion integrals. At last the case of complete spontaneous SU(3) symmetry breaking, at that the Hamiltonian possesses SU(3) symmetry. For all mentioned cases nonlinear dynamic equations are obtained and spin waves specters are established.

Thermodynamics of small electromagnetic generators, an experimental perspective

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The fabrication of relatively small electromagnetic generators has been reported recently in the literature by a number of research groups. Their characteristic sizes are on the order of one millimeter. With proper tune up, these devices have been used to convert waste ambient vibration noise into useful electric power. We would like to discuss the possibility of reducing the size of the generator to nanometer scale allowing the observation and manipulation of individual thermodynamic degrees of freedom. We present preliminary experimental results.

Stochastic resonance, synchronization and transport in systems driven by Lévy noises

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A standard approach to analysis of noise-induced effects in stochastic dynamics assumes a Gaussian character of the noise term describing interaction of the analyzed system with its complex surroundings. An additional assumption about the existence of timescale separation between the dynamics of the measured observable and the typical timescale of the noise allows external fluctuations to be modeled as temporally uncorrelated and therefore white. However, in many natural phenomena the assumptions concerning the abovementioned properties of "Gaussianity" and "whiteness" of the noise can be violated. In this context, so called Lévy flights correspond to the class of Markov processes which still can be interpreted as white, but distributed according to a more general, infinitely divisible, stable and non-Gaussian law. Lévy noise-driven non-equilibrium systems are known to manifest interesting physical properties and have been addressed in various scenarios of physical transport exhibiting a superdiffusive behavior.

In order to document and discuss the widespread presence in nature of the stochastic resonance phenomenon, we investigate the generic double-well potential model perturbed by the α-stable Lévy type noises. Our research focuses on the analysis of the influence of noise parameters on a shape of SR measures, revealing presence and robustness of the SR in the system at hand. In addition to the discussion of the SR, a brief summary of stochastic dynamics under the influence of Lévy white noise perturbations will be given. In particular, problems of synchroznization and directed transport (ratcheting effect) will be covered.

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Superfluid state of magnetoexitons in double layer graphene structures

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The possibility of realization of a superfluid state of bound electron-hole pairs (magnetoexitons) with spatially separated components in a graphene double layer structure (two graphene layers separated by the dielectric layer) subjected by a strong perpendicular to the layers magnetic field is analyzed. The flow of such pairs is equivalent to two counterflow electrical currents in the layers.

In graphene the energies of the Landau levels are given by the expression $E_n = \sqrt{2n}\hbar v_F/\ell$, where $v_F \approx 10^8$ cm/s is the parameter of the electron structure, $\ell = \sqrt{\hbar c/eB}$ is the magnetic length, and $n = 0, \pm 1, \pm 2, \ldots$. In undoped graphene the 0-th Landau level is half filled. We show that an imbalance of filling factors of the layers $\nu_i^{(0)}$ is required to achieve the superfluid state of magnetoexitons (the filling factors $\nu_i^{(0)}$ are defined as the fraction of occupied states in the 0-th Landau level times the spin and valley degeneracy factor $g = 4$). The imbalance can be created by an electrostatic field (gate voltage) applied perpendicular to the layers.

We compute the critical interlayer distance d_c and the superfluid stiffness versus the filling factor imbalance. The maximum superfluid stiffness is achieved for the filling factors $\nu_1^{(0)} = 5/2$, $\nu_2^{(0)} = 3/2$ and $\nu_1^{(0)} = 7/2$, $\nu_2^{(0)} = 1/2$, while the critical distance at such filling factors is minimal (the inequality $d < d_c$ yields the condition of stability with respect to appearance of charge density waves). The spectrum of collective excitations is computed and the dependence of the Berezinskii-Kosterlitz-Thouless transition temperature on the imbalance of the filling factors and on the interlayer distance is found. The case of large gate voltage, when in one layer the $n = 1$ level becomes partially filled and in the other layer the $n = -1$ level becomes partially unfilled, is also analyzed.

The advantages of use graphene double layers instead of double quantum well GaAs heterostructures are discussed. In graphene systems much smaller tunneling between the layers reduces considerable the energy losses. Beside that, lower magnetic fields are required to achieve the superfluid state of magnetoexitons in graphene systems.

Memory effects in a non-equilibrium Langevin equation describing effective cooling via feedback currents

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The possibility of measuring low-temperature signals by subjecting the analyzed source to an active feedback scheme has attracted a lot of interest in recent times. This is achieved driving the interaction between the measuring apparatus and the observed system out of equilibrium, through constantly recycling the currents induced by the latter on the former. The delay line produces an effective dissipation within the source-apparatus universe, beyond the constraints dictated by the Fluctuation and Dissipation Theorem. It is *as if* the source now operates at temperatures lower than the actual bath temperature. This technique has been applied successfully to – among others – diverse systems such as nano-mechanical oscillators and gravitational wave detectors. We have analyzed a Langevin model of the feedback effect. The feedback current adds a memory term to the equilibrium equation of a dumped oscillator, driving the circuital currents and charges of the measuring apparatus out of their equilibrium with the source. If the source is purely thermal, we can calculate explicitly the power spectrum of the current. One can show that for high quality factors the power spectrum of the current generated by the Langevin equation is (unsurprisingly) *almost* a Lorentzian curve, with effective dissipation, as if the system equilibrates at a modified temperature. Less obvious, the resonance frequency also depends on the feedback gain, due to the memory effect. We also show substantial deviations from such behavior, illustrating that equilibrium-like descriptions would be entirely erroneous in certain conditions. The system in fact behaves in a qualitatively different way in those circumstances, leaving no room for 'effective' adjustments. This apparently depends on the peculiar nature of oscillators with low quality factors.

WWW page `http://www.rarenoise.lnl.infn.it`

Nonequilibrium entanglement entropy of quantum spin chains

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We consider a quantum spin chain (such as the Ising chain in a transverse field of strength h) at $T = 0$ which is divided into two parts, $\mathcal{A}$ and $\mathcal{B}$. The interaction of the system is suddenly changed: for time $t > 0$ the system is at the quantum critical point, and measure the time evolution of the von Neumann entropy, $\mathcal{S}_\mathcal{A}(t)$. We consider different type of quenches and obtain different type of asymptotic time-dependence.

i) For a *global quench* of the control parameter of the homogeneous chain we obtain analytically [1]:

$$\mathcal{S}_\mathcal{A}(t) = \alpha(h)t.$$

ii) Quenching out a gradient field: $h_i = 1 + gi$, we have [1]:

$$\mathcal{S}_\mathcal{A}(t) \sim gt^2.$$

iii) For a *local quench* of an interface defect [2]:

$$\mathcal{S}_\mathcal{A}(t) = \frac{2c_{eff}}{3} \log t,$$

with c_{eff} is the effective central charge.

iv) For a *local quench* in a disordered chain [3]:

$$\mathcal{S}_\mathcal{A}(t) = \frac{c_{eff}}{3} \log\log t.$$

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Liquid-gas phase behavior of polydisperse dipolar hard-sphere fluid

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Liquid-gas phase diagram for the dipolar hard-sphere fluid was calculated theoretically more than thirty five years ago by Rushbrooke et al. [1]. According to these calculations the critical point is located at reduced temperature $T_c^* = 0.279$ and reduced density $\rho_c^* = 0.159$. Systematic computer simulation search for the liquid-gas phase coexistence was initiated only twenty years later [2,3]. These investigations were carried out at a temperatures well beyond predicted theoretically, however no evidence for the phase transition was found. Shortly after there appeared a number of the theoretical papers, in which the arguments were given as to why the existence of the liquid-gas phase transition has to be ruled out. It was suggested that due to the highly anisotropic character of the dipole-dipole interaction the formation of the chains in the 'nose-to-tail' arrangement suppresses the liquid-gas phase transition. However, recent computer simulation [4], carried out for the temperatures lower than those studied earlier, presented the evidence for the phase transition with the critical point located at $T^* \approx 0.15 - 0.16$ and $\rho^* \approx 0.1$.

We present and discuss the liquid-gas phase diagrams of the monodisperse and polydisperse versions of the dipolar hard-sphere fluid, calculated using thermodynamic perturbation theory for associative fluids with center-center type of interaction [5,6].

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The surface tension of small drops

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An effective method of nanoparticles production is the condensation of nanodrops from supersaturated vapor. Nucleation, formation of critical nuclei, is the first stage of such condensation. The surface tension of small drops is the most impotent parameter in the nucleation theory, as it determines the work of the critical nuclei formation.

In our report the results of molecular dynamics calculations of small drops are presented. The equilibrium states of Lennard-Jones molecular system containing one small drop of $50 - 4000$ molecules and the saturated vapor have been prepared. The density profiles, the Irving-Kirkwood pressure tensors, the chemical potentials of the systems, the mechanical and Gibbs's surface tensions have been calculated. The difference between the mechanical definition of surface tension and the Gibbs's one is in the fact, that in the first case the real drop is replaced by the spherical container, the pressure inside the container being chosen as equal to the pressure in the center of the drop, and in the second case the pressure inside the container corresponds to the pressure in the bulk liquid with chemical potential equal to that in the calculated system.

The dependence of the surface tension of small drops on the equimolar radius and temperature has been calculated. It was found that the mechanical surface tension is different from the Gibbs's surface tension for drops of $50 - 2000$ molecules and is equal for drops of more than 2000 molecules. It is shown that both the mechanical and Gibbs's surface tensions decrease with the decrease of the equimolar radius of the drop, and reach zero at the same R_0 depending on temperature. The dependence of the ratio of the surface tension of the drop to the surface tension of the flat surface liquid-vapor (σ/σ_∞) on the ratio of the equimolar radius of the drop to R_0 is a universal function.

To a question on application of the statistical theory for the description of industrial systems

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The application of the methods of Statistical Physics for its description is possible owing to the representation of the manufacturing firm with mass production output as a system with large number of elements (the basic products) of stochastic nature, which are in the production process. The behavior of the basic products along the technological chain depends on the definite manufacturing and technological laws in accordance with the technological process of the manufacturing firm, its production plan, the availability of manpower resources and equipment. The state of the production system's basic products at any instant of time is given as the point in two-dimensional phase space. The function of the basic product's distribution in the rate of expense's variation is set and the equation similar to the kinetic equation in Physics is written down. The engineer-production function, which is analogous to the force moving the basic product along the technological chain of the production process, is set and can be determined from the technical documentation of the manufactured article approved in the manufacturing firm. The producer function, that describes the interaction of the basic products (the system's elements) during their moving along the technological chain of production process with technical equipment, is based on the equipment disposition schemes and its technical characteristics according to operating mode of half-finished products. Using the kinetic equation a closed system of balances equations is written down in a zero approximation on a small parameter for the moments of distribution function. The system of balances equations describes the behavior of the basic economical macroscopic quantities of the production system, such as reserve, pace and dispersion of the production output along the technological chain. From the balances equations were obtained the well-known relations in business operation theory for calculation of reserves and paces of the production output.

Dipole glass phase in ferro-antiferroelectric mixed systems

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The problem of microscopic description of dipole glass phase in ferro-antiferroelectric mixed systems is discussed. The dipole glass order parameter as well ferroelectric and antiferroelectric order parameters are constructed on the base of pair and single correlation functions for nearest neighbours particles [1].

The phase under investigation take place at low temperature for intermediate values of concentration and change the behaviour of it's pair distribution function in several points [2]. Phase diagram and some thermodynamic functions of mixed system are obtained and analyzed.

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Dielectric function for a semi-infinite metal

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Investigating of the interacting electronic subsystem of metal is one of the central problems of solid state physics. It is caused by that the electronic subsystem plays a main role in formation of the basic characteristics of a metal crystal, such as its structure, binding energy, phonon spectrum, electromagnetic properties. Research of interacting electronic subsystem in itself is difficult, and in case of the semi-infinite metal considered by us becomes more difficult because the electronic subsystem is very nonuniform near a metal surface.

In non-bounded metal the screening properties of the interacting electronic subsystem, and also dispersion of plasmon oscillations are defined by dielectric function $\varepsilon(\mathbf{q},\omega)$, which is a scalar function of a three-dimensional wave vector $\mathbf{q}$ and frequency ω. In contrast to non-bounded metal the dielectric function, owing to presence of a flat surface of metal, is not a scalar function, and is a matrix function $\varepsilon_{k_1,k_2}(\mathbf{q},\omega)$, here $\mathbf{q}$ is two-dimensional wave vector responsible for expansion of Fourier in a plane parallel to the surface, k_1 and k_2 are responsible for expansion of Fourier perpendicularly to the surface. We have proposed an approach to calculation of dielectric function taking into account correlation effects in approach which is similar to local field corrections in the theory of homogeneous electronic gas. Efficiency of this approach is illustrated by calculations of static ($\omega = 0$) dielectric function and effective potential of interelectronic interaction. It is shown, that the offered approach correctly considers the image forces.

Semi-infinite metal: thermodynamic characteristics and effective pair interionic potentials

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Theoretical studies of equilibrium properties of a metal surface is very difficult, because an electronic subsystem of bounded metal is very spatially nonuniform. It essentially complicates the consecutive account of many-particle effects in an electronic subsystem. The greatest successes in studying of electronic properties of a metal surface have been attained within density functional theory (DFT). However the study of properties of a metal surface which are caused by discreteness of the ionic subsystem is problematic, as method of constructing necessary energy functionals is not known.

In presented work systematic perturbation theory for bounded metals, described by nonlocal pseudo-potentials, is developed. The semi-infinite jellium [1,2] is used as the reference system and the perturbation theory with respect to the "difference potential" (that is the difference between the pseudo-potential of ions and the electrostatic potential of the semi-infinite jellium positive background) is constructed.

Potentials of the interionic interaction has been great interest both for this theory and for atomistic modeling of materials [3]. We investigate potential of pair interionic interaction in the semibounded metal with use of different local field corrections.

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Relationships between electron band filling and type of charge and magnetic order

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Charge and spin orderings are studied on the infinite square lattice (ground state) and on the 4×4 cluster (finite temperatures) within the generalized Falicov-Kimball model with Hund coupling between localized and itinerant electrons. Using the restricted phase diagram method (RPDM), a number of simple rules of formation of various sorts of ground state phases are detected. In particular, relationships between density of current carriers (electrons or holes) and type of charge and magnetic arrangement are determined. In the mixed valence regime only axial (vertical or horizontal) stripes are found for intermediate values of the coupling constants. They are composed of ferromagnetic or antiferromagnetic chains interchanged with nonmagnetic ones. For band fillings close to the half filling, stripe phases oriented along one of the main diagonal direction are formed. The results suggest a possibility of tuning modulations of charge and magnetic superstructures with a change in doping.

Finite temperature properties of the model are examined by direct diagonalization of the Hamiltonian for the finite 4×4 cluster at the half filling. Magnetization, specific heat and susceptibility versus temperature and magnetic field are presented and compared to the characteristics calculated by other authors, as well as to some experimental data.

Adsorption of model electrolytes in disordered porous materials. Predictions of the replica integral equation theory

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Partitioning of electrolytes between matrices containing charges and the bulk solution is not only a matter of academic interest, but finds its practical application in many technological, industrial and biological processes (for example: desalination of water, ion exchange, membrane equilibria etc.).

The present contribution will show that the replica Ornstein–Zernike integral equation theory is an adequate theoretical tool for studying preferential adsorption of a mixture of model electrolytes in random matrix media. The latter will be considered as a quenched equilibrium distribution of a size and charge symmetrical electrolyte, while the electrolyte that will be allowed to anneal within the matrix particles will be represented as a mixture of two electrolytes with common ion (for example AX and BX, where A and B are cations that differ in size and/or charge and X is the common anion).

After a short conceptual introduction to the replica theory its predictions will be compared with the exact results obtained by the Monte Carlo simulations in the grand canonical ensemble. It will be shown that the theory is in good agreement with the simulation.

Next, we will present a phase diagram for the given model. We will see that sorption of the electrolyte into the matrix media occurs only at low matrix concentrations and at low concentrations of the annealing electrolyte, whereas at higher concentrations we get exclusion from the porous media.

Ions with smaller radii (*i.e.* larger surface charge density) tend to be preferentially absorbed, since they can come closer to the matrix ions and feel stronger Coulombic force. Replica Ornstein–Zernike theory seems to be appropriate for studying the dependence of different parameters (matrix preparation, concentration, conditions of annealing) on the preferential adsorption of ions from such mixtures.

Magnetic properties of a strongly correlated system on the Bethe lattice

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The Green's function and equations of motion formalism allows one to exactly solve a large class of models useful for the study of strongly correlated systems. In this article, we study the influence of an external magnetic field h on the phase diagram of a system of Fermi particles living on the sites of a Bethe lattice with coordination number z and interacting through onsite U and nearest-neighbor V interactions. This is a physical realization of the extended Hubbard model in the atomic limit. Our results establish the existence of different phases in the three dimensional spaces (U, T, h) and (n, T, h) – where n is the filling – with relative phase transitions, as well as different types of charge ordering. The magnetic field may dramatically affect the critical temperature below which a long-range charge ordered phase is observed, as well as the behavior of thermodynamic quantities, inducing, for instance, magnetization plateaus in the magnetization curves. Relevant thermodynamic quantities – such as specific heat, susceptibility, entropy – are also investigated at finite temperature as functions of the on-site potential, particle density and of the magnetic field.

Excitonic states in double-walled carbon nanotubes

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A simple model for investigation of on-tube and inter-tube exciton states in (n,0)@(m,0) double-walled carbon nanotubes is proposed. The exciton contributions to optical spectra of such tubes are described within this model.

Nonequilibrium statistical operator in the generalized molecular hydrodynamics of liquids

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The investigations of nonequilibrium processes in classical and quantum systems far from equilibrium, which are characterized by their own lifetime (relaxation time), are actual in modern theory for nonequilibrium processes. Taking into consideration that definite nonequilibrium statistical operator corresponds to the state of molecular hydrodynamics the question for considerations beyond the framework of molecular hydrodynamics arises. Using new interpretation of the Zubarev nonequilibrium statistical operator (NSO) method, in which operation of taking of invariant part in NSO is treated as averaging of quasiequilibrium statistical operator on distribution of past lifetime of system, we construct a nonequilibrium statistical operator and derive the corresponding transport equations for a system that relaxes and passes into the state of molecular hydrodynamics. Deriving the equations an explicit dependence of the NSO on time was taken into account. By the structure of memory functions, transport equations involve second-order terms with respect to time-correlation functions. Together with the nonequilibrium statistical operator, they can describe nonequilibrium processes connected with the relaxation of the state of a system of interacting particles to the state of molecular hydrodynamics. The equations describing the time-correlation functions and corresponding to the system of transport equations are important. According to the structure of memory functions, they must be constructed for the extended set of dynamical variables.

New approach for calculation of elastic fields of quantum dots in semi-infinite matrices with Green's functions formalism

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We present new calculation approach and analytical equations based on Green's function formalism, which are used to calculate elastic fields produced by a quantum dot buried in a semi-infinite matrix with a rigid surface. The dot of an arbitrary shape as well as quantum dot arrays can be very efficiently carried out within the presented technique. This technique can be exploited for matrices with weak electromechanical coupling where it is suitable for arbitrary electrical boundary conditions applied at the surface. Approach of this work is much easier and faster than other existing methods based on Green's function formalism for this problem. It allows one substantially reduce computation time and make it comparable with the computation time needed for simple infinite-matrix calculations. In the framework of the method proposed here we present calculations of elastic fields for $Ge_{(1-x)}Si_{(x)}$ pyramidal and cubic QDs in semi-infinite Si matrix with rigid surface. Resulting strain distributions were proved to reach asymptotical behavior far from the surface and show additional strain accumulation near the surface. These results were published in Journal of Applied Physics (JAP-2009, v. 105, p. 023525).

Influence of the temperature-dependent electron-energy spectrum realignment on the formation of homogeneous magnetic short-range-ordered regions in disordered b.c.c. alloys

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Formation of the homogeneous magnetic short-range-ordered regions in disordered b.c.c. alloys under the influence of the electron-energy spectrum realignment with a temperature is considered. For the description of electron states in a crystal, the multiband model of a tight binding and the developed method for the cluster expansion for Green's functions and thermodynamical potential of a disordered crystal are used. Within the scope of the mentioned approach, the calculations of both the electron-energy spectrum and the temperature dependence of equilibrium values of the pair-wise magnetic-correlation parameters of disordered b.c.c.-$Fe_{0.5}Co_{0.5}$ alloy are performed. The equilibrium values of parameters of magnetic and interatomic correlations are obtained from the condition that a free energy is minimal. Strong correlations between electrons in conditions of their strong Coulomb repulsion and the well-developed short-range order of substitutional atoms lead to appearance of a quasi-gap in the electron-energy spectrum. The microscopic mechanism of magnetic ordering in a b.c.c. alloy is concerned with both the Fermi-level position within the quasi-gap region and the realignment of the electron-energy spectrum with a change of temperature. The parameters of pair-wise magnetic correlations decrease with the temperature increase that leads to increasing electron density of states at the Fermi level. The equilibrium parameters' values of the pair-wise magnetic correlations at some temperature allow to calculate the respective linear sizes of homogeneous magnetic short-range-order regions in b.c.c. alloys. The result of computation for b.c.c.-$Fe_{0.5}Co_{0.5}$ alloy—namely, a steadily decreasing temperature dependence of the linear sizes of homogeneous magnetic-order regions—conforms to the experimental data obtained by Yu.I. Ustinovshchikov et al.(2003).

Photon kinetics in plasmas

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We present a kinetic theory of radiative processes in many-component plasmas with relativistic electrons and nonrelativistic heavy particles. Using the non-equilibrium Green's function technique in many-particle QED, we show that the transverse field correlation functions can be naturally decomposed into sharply peaked (non-Lorentzian) parts that describe resonant (propagating) photons and off-shell parts corresponding to virtual photons in the medium. Analogous decompositions are obtained for the longitudinal field correlation functions and the correlation functions of relativistic electrons. We derive a kinetic equation for the resonant photons with a finite spectral width and show that the off-shell parts of the particle and field correlation functions are essential to calculate the local radiating power in plasmas and recover the results of vacuum QED. The influence of plasma effects on radiative processes is discussed.

Thermodynamics of lattice model of intercalation

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The thermodynamics of the lattice model of intercalation of ions in crystals is considered in the mean field approximation. Pseudospin formalism is used in describing the interaction of ions with electrons. The effective attractive interaction between ions is formed due to the pseudospin-electron interaction and the condition of the appearance of phase transition of the first order with jumps of the ion and electron concentration is established (in the regime of the fixed concentrations it corresponds to the phase separation). This interaction also leads to the shift of the electron band positions. It is found that the total capacity of the system increases near phase transition point. The influence of impurities on these transitions and electrostatic capacity of the system is investigated. The possibility of hopping of intercalated ions between different positions is taken into account. The existence of the phase with $\langle S^x \rangle \neq 0$ was revealed (this phase is an analog of superfluid phase in the systems of hard-core bosons). The possibility of phase transitions of the first and second order to the modulated phase is revealed. Phase diagrams in the plane the chemical potential of the ions-parameter of the ion transfer are built. It is shown that at high values of the parameter of ion transfer, the phase transitions with jumps of the ion and electron concentrations disappear.

Gas-liquid critical point in model ionic fluids with charge and size asymmetry

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The phase and critical behaviour of ionic fluids has long been a topic of great interest. A lot of efforts have been made to obtain the phase diagrams and calculate the locus of the gas-liquid (GL) critical point even for the simplest model of ionic fluids, the so-called restricted primitive model, in which monovalent equi-sized hard spheres interact via the Coulomb potential. The studies of the effects of asymmetry on the GL phase diagram of the size- and charge-asymmetric primitive models (PM) have been recently started using both the computer simulations and theoretical methods. Comparison of simulated critical parameters and theoretical predictions has revealed that several established theories, such as the mean spherical approximation are unable to predict the trends observed in simulations, particularly with regards to the decrease of the critical temperature and critical density with increasing size asymmetry [1,2].

We develop the theoretical approach to the study of the GL phase behaviour of the size- and charge-asymmetric PM. The model is characterized by the two parameters: diameter-, $\lambda = \sigma_+/\sigma_-$ and charge, $z = q_+/|q_-|$, ratios of the two ionic species. The approach allows us to derive the exact functional representation of the grand partition function and formulate, on this basis, the perturbation theory. First, we perform the stability analysis in the Gaussian approximation. This leads us to the trends for the critical parameters consistent with [3]. Then, we study the GL critical point of the PM taking into account the correlation effects of higher order. We calculate binodal curves and critical parameters as functions of λ and z and compare our results with those obtained by the theory and computer simulations.

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About mutual influence of transport processes and inner structure in condensed media

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Results of analysis of condensed media with anisotropic structure elements are presented in the report. Thermodynamics and nonequilibrium processes in such systems are described by additional physical values. The initiation and formation of spatial structures and their self organization in condensed media are possible thanks to chemical, radiation, ecological or biological transformations taking into account diffusion processes in such distributed systems.

The base of present research is Hamilton's approach. The mutual influence of the form and size of structure elements of medium on the mass transport processes are traced in detail. Conformational degrees of freedom are introduced as definite functions of distortion tensor. The full set of Poisson brackets for all the set of macroscopic values is obtained and nonlinear dynamic equations taking into account relaxation processes are introduced. General structure of dissipative flows is found and the possibility of existence of additional kinetic coefficients, which describe new mechanisms of relaxation in a medium, connected with inner structure presence is shown. Solutions of mentioned nonlinear equations in stationary and nonstationary cases in conditions with different geometry are obtained and their physical interpretation is given.

Non-equilibrium spin dynamics in dilute magnetic semiconductor under optical polarization spin of electrons and carrier-warming electric field

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In this paper we present the new results of theoretical studies concerning the action of carrier-warming electric field on non-equilibrium spin polarization of the electrons in a diluted magnetic semiconductor with parameters of n-InP:Fe. We considered a sample illuminated by a circular polarized light with a frequency satisfying the condition of impurity absorption. The dynamics of the carriers was described by one-dimensional system of non-linear differential equations in partial derivatives, including the continuity equation for spin-polarized electrons in conductivity band and at the impurity level, as well as the Gauss law. We investigated the evolution of phase portraits of the system, maximum Lyapunov exponent and Hausdorff dimension as functions of applied electric field. It was found that the space-time distributions of band electron concentration and their spin polarization degree could be represented as a superposition of high- and low-frequency harmonics with different amplitudes. The system studied proved to be stable towards the variation of the external factors. Depending on the applied field and other control parameters, the electron system studied can be efficiently switched between five possible stable states. Alternatively, it may be forced to stay in five-times degenerated state, deterministic state, or quasi-chaotic state. The results obtained offer important insights for the construction and optimization of spintronic devices based on diluted magnetic semiconductors.

Lifshitz points: Recent theoretical progress

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Lifshitz point (LP) is a special multicritical point, which typically appears in strongly anisotropic systems. An example can be provided by the ANNNI (axial next-nearest neighbor Ising) model with competing ferro- and antiferromagnetic interactions along a singled-out direction where the uniaxial LP is realized. Such spin model systems are well suited for numerical Monte Carlo simulations. Experimentally, LPs have been observed in a number of quite different physical systems. Among them, the best studied material is the magnetic metallic compound MnP.

Recently, the physical properties associated with this special point have been the subject of extensive investigations. Our aim is to give a short review of the critical behavior at LPs and to present the new achievements of its theoretical studies.

First we show the main results of our renormalization-group analysis of the bulk properties of d dimensional systems at m-axial LPs with generic $m \in [0, d]$ by means of an $\epsilon{=}4{+}m/2{-}d$ expansion carried out up to order $O(\epsilon^2)$. LP's critical exponents could also be obtained in the $1/N$ expansion covering the whole accessible region of d, while the large number N of the order-parameter components is taken into account to order $O(1/N)$. Shown to be equivalent in the overlapping regions of validity of these two different approaches, our results resolve a longstanding controversy in a series of previous publications.

At LPs, the question of relevance of spatial anisotropies in m modulation directions is not trivial. We show that they can influence the critical behavior at LPs, in contrast to usual critical points. Another special feature discussed is that the surface properties of bounded systems are different at LPs, depending on the orientation of surfaces with respect to the modulation axes. Finally, we give a taste of fluctuation-induced forces appearing in strongly anisotropic systems at LPs.

The work has been done in collaboration with H. W. Diehl, M. Burgsmüller (Germany), Yu. M. Pis'mak, P. V. Prudnikov (Russia), R. K. P. Zia (USA).

Correlation effects in the model of orbitally degenerate electronic subsystem of fullerides: the configurational representation of Hamiltonian

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Despite the intensive experimental and theoretical studies, the diversity of physical properties of doped fullerides remains unexplained at a microscopic level. Doped systems A_3C_{60} (where A=K,Rb,Cs) turn out to be metallic at low temperatures. According to the theoretical band structure calculations (see [1] for review), fullerides with integer band-filling parameter n should be Mott-Hubbard insulators by electric nature, because all of them possess large enough values of intra-atomic Coulomb correlation parameter U. At the same time, in some of the doped fullerides (for example, AC_{60} and A_3C_{60}) a metallic state of unclear nature is realized. The present study is devoted to investigation of electrical and magnetic properties interplay in electronic subsystem of fullerides with strong electron correlations. In our study a model of doped fulleride electronic subsystem is formulated with taking into account the orbital degeneracy, strong intra-atomic correlations and the correlated hopping of electrons. The importance of proper accounting for these interactions is caused by a competition between on-site Coulomb correlation (characterized by Hubbard parameter U) and delocalization processes (translational motion of electrons is determined by bare bandwidth and energy levels degeneracy), which a realization of the insulating or metallic state depends on. Model Hamiltonian configurational representations for description of doped fullerides has been built. On a basis of the analysis carried out we argue that for an explanation of a metallic behavior of Mott-Hubbard system (x=3 corresponds to the half-filled conduction band) three-fold degeneracy of energy levels and Hund's rule coupling has to be properly taken into account. The possibility of metal-insulation transition in the system in the framework of the proposed model, is discussed.

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Self-organization processes at exciton condensation in quantum wells

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A theory of exciton condensation in semiconductor double quantum wells is presented. By applying an electric field to the double quantum well, it is possible to force electrons and holes to different wells. As the result the exciton lifetime becomes by several order of magnitude longer than the lifetime of excitons in the bulk material. This circumstance allows creation of a large exciton density in order to study processes of exciton-exciton interaction. It is assumed that a condensed phase of excitons arises due to some (exchange) exciton-exciton attractive interaction and is described by several parameters. Non-equilibrium conditions, caused by finite value of exciton lifetime and a presence of pumping, are taking into account. For description of spatial distribution of condensed and gas phases two models of phase transitions are used: the model of nucleation and growth and the model of spinodal decomposition generalized on unstable particles. It is shown that due to finite value of the exciton lifetime the sizes of condensed phases are restricted and in two-dimensional case regions of condensed phase have a form of islands situated among excitonic gas. The structure arises due to an interaction between condensed phase islands through exciton concentration fields. The evolution of the islands of condensed phase with changing the temperature, pumping is studied. The theory is applied for the explanation of different periodical structures in luminescence spectra which were observed in several experiments last years. The influence of different type of external potential (for example, due to a presence of a window, slot in metallic electrode, so on) on the periodical structures is considered. It is shown that appearance of the structures occurs due to the non-equilibrium state of the system caused by the finite value of the exciton lifetime and the presence of pumping, and, therefore, it is the result of self-organization processes in a non-equilibrium system.

Permutation group theory in construction of Feynman diagrams for mass operator of interacting electrons and electrons interacting with phonons

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The double permutation method is developed for construction of Feynman diagrams for mass operator of interacting electrons. The derived expression allowing to separate classes of permutations (Young diagrams) corresponding to disconnected Feynman diagrams, which are not taken into consideration. The criteria stated here allow omitting the permutations corresponding to disconnected and improper diagrams, depending to other classes of DPs. The other criterion is stated to avoid the repetitions of the same diagrams, denoted by different permutations (as result of different numbering of nodes). All these statements allow reducing the number of considered permutations sufficiently: from 24 to 6 and from 720 to 42 in the second and the third orders of perturbation theory. The symmetrical analysis of permutations is carried out. It allows avoiding the pairs of asymmetrical diagrams, corresponding to the same analytical expressions. Using this method Feynman diagrams for mass operator of electrons in the second and the third orders of perturbation theory are constructed. The developed method can be used as basis for algorithm of construction of Feynman diagrams for mass operator in high orders of perturbation theory.

Double permutation method is used for Feynman diagram construction for mass operator for electron-phonon interaction. The derived expressions for DPs and phonon components allow constructing the diagrams automatically. To avoid repetition of asymmetric diagrams, which correspond to the same analytical expression, we introduce the procedure of inversion in phonon component, and identify symmetric and pair of asymmetric phonon components. For every type of DP (denoted by its digital encoding), taking into account its symmetry, we perform set of transformations on this DP, list all DPs of the type and all corresponding Feynman diagrams of mass operator automatically. It is clear that no more expressions (diagrams) for the concerned order of perturbation theory for mass operator can be designed.

Peculiarities of diffusion of particles on disordered lattices

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A system of particles on periodic two- or three dimensional lattices with uniform site energies is considered. Particle jumps to nearest neighbor vacant sites are thermally activated with randomly distributed intersite barriers. The statistical mechanics expressions for the kinetic diffusion coefficient that take into account interparticle interactions are derived for dynamically disordered systems.

The lattice systems with uniform, exponential and Gaussian probability distributions of the barriers are investigated.

The comparison between analytical results and Monte Carlo simulation data shows that the equilibrium characteristics of the model (the chemical potential and the probability for two nearest neighbor lattice sites to be vacant) are represented by the diagram approximation with high accuracy.

For the systems with static disorder the analytical expressions for the kinetic diffusion coefficient at low and high temperatures are proposed and investigated. The interpolation expression for the case of intermediate temperatures is considered.

The activation energy U_J for the kinetic diffusion coefficient is suggested to be described by the following expression

$$U_J = \epsilon_0 - (\epsilon_0 - \epsilon_p)\exp(-k_{\mathrm{B}}T/\epsilon_J), \tag{1}$$

where ϵ_J depends on the type of lattice system and probability distribution functions $\nu(\epsilon)$ of the barriers and can be determined from MCS data; T is temperature; k_{B} is the Boltzmann constant; ϵ_0 is the average barrier energy; ϵ_p is the percolation energy that is calculated in accordance with the following expression

$$\int_0^{\epsilon_p} \nu(\epsilon)d\epsilon = p_c, \tag{2}$$

where p_c is the threshold for the bond percolation problem.

Modeling the phase transition kinetics in lattice systems

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For considering the density evolution of a lattice fluid the non-equilibrium distribution in a local equilibrium representation is used. The non-equilibrium distribution function is determined by local values of the chemical potential at lattice sites. The expressions in terms of the transition probabilities for microscopic fluxes between lattice sites and the balance equations are used for formulating the evolution equations of inhomogeneous systems in finite differences. The simplest Euler's numerical algorithm is used for integrating these equations over time. This algorithm ensures stable solution of the equations at little requirements for computational resources that permitted to investigate phase transition kinetics at various thermodynamic, initial and boundary conditions.

The lattice fluid with nearest neighbor interparticle attraction on square and simple cubic lattices below critical temperature is considered. The initial density distribution is taken to consist of two regions: the high density region around the center of the system with density slightly lower equilibrium liquid density and the low density region outside the central region with density slightly higher the equilibrium gas density at a given temperature. The average system density corresponds to thermodynamically unstable state at subcritical temperature and the high density region serves as a region for the liquid density phase formation (inoculating area).

In two-dimensional systems the second high density region on the system periphery appears that disappears at bigger times. The inoculating area critical size is approximately equal to the double width of the phase transition region. Several complementary condensed areas in three-dimensional systems are observed. Number of areas depends on initial conditions. However, as opposed to two-dimensional systems, phase stratification takes place with arbitrary inoculating area size.

For the charging process imitation of a battery the first two lattice layers are initially filled above the condense phase concentration and the other layers are empty. The concentration profile kinetics in the system with and without external electric field are investigated.

Steady-state molecular dynamics simulation of vapour to liquid nucleation with McDonald's dæmon

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Scientifically, the most interesting step of condensation is the droplet formation up to the critical size. In a closed system, this is an instationary process, as the vapour is depleted by the emerging liquid proto-phase. This imposes a limitation on direct molecular dynamics (MD) simulation of nucleation by affecting the properties of the vapour to a significant extent so that the nucleation rate varies over simulation time.

A new molecular simulation method for sampling both nucleation kinetics and steady-state properties of a supersaturated vapour is introduced in the present work. The idea behind the new approach is to simulate the production of droplets up to a given size for a specified metastable state. This is achieved by combining grand canonical MD and an ≪intelligent being≫ that continuously removes all large droplets: McDonald's dæmon [Am. J. Phys. 31 (1962): 31]. In this way, nucleation is studied by a steady-state simulation.

A series of simulations at temperatures between 0.7 T_3 and 0.9 T_c, where T_3 and T_c are the triple point and critical temperature, respectively, is conducted for the truncated and shifted Lennard-Jones fluid which accurately describes the fluid phase coexistence of noble gases and methane. A comparison to canonical ensemble MD simulation as well as Monte Carlo simulation with forward flux sampling confirms the viability of the new method. The classical nucleation theory is found to underpredict the nucleation rate by two orders of magnitude and to overstate the free energy of droplet formation.

Bose condensation in (random) traps

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We study a condensation of the perfect Bose-gas in the presence of random external potentials. It is shown that a generalised condensation (*à la* van den Berg-Lewis-Pulé) in the one-particle random eigenstates occurs *if and only if* it implies the occupation of one-particle kinetic-energy eigenstates corresponding to the generalised condensation in the free Bose-gas. We also prove that the amounts of the both condensate densities are *equal*. Our method is based on an explicit estimate of the particle occupation measure in the one-body kinetic-energy eigenstates for non-interacting disordered boson systems. It allows also to re-examine the properties of the perfect Bose-gas in the presence of the *scaled* random and non-random traps, for which we prove the similar results.

New mean field approximation in the theory of strongly correlated systems

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Approach which develops ideas of papers [1–3] is proposed. In framework of the proposed approximation the single electron Green function for the Hubbard model is obtained, in particular. This function for the case of half filled band (mean number of electrons per site $n = n_\uparrow = n_\downarrow = 1$) and absence of the magnetic ordering has the following form

$$G_{\mathbf{k}} = \frac{1}{4\pi}\left(\frac{A_{\mathbf{k}}}{E - E_1(\mathbf{k})} + \frac{B_{\mathbf{k}}}{E - E_2(\mathbf{k})}\right),$$

where $A_{\mathbf{k}}$ and $B_{\mathbf{k}}$ depend on the energy parameters $t(\mathbf{k})$ (hopping integral) and U (intraatomic Coulomb repulsion) as well as on the polar states concentration d (concentrations of doublons and holes are equal),

$$E_{1,2}(\mathbf{k}) = \frac{(\epsilon_1 + \epsilon_2)}{2} + (1 - 2d)t(\mathbf{k}) \mp \frac{1}{2}\sqrt{(U + \epsilon_2 - \epsilon_1)^2 + (4dt(\mathbf{k}))^2},$$

$$\epsilon_1 = \frac{n_\downarrow}{N}\sum_{\mathbf{k}} \frac{t^2(\mathbf{k})}{E - \frac{U}{2} - t(\mathbf{k})}, \quad \epsilon_2 = \frac{n_\uparrow}{N}\sum_{\mathbf{k}} \frac{t^2(\mathbf{k})}{E + \frac{U}{2} - t(\mathbf{k})}.$$

Two latter expressions are written with taking into account possible magnetic ordering ($n_\uparrow \neq n_\downarrow$) in presense of magnetic field. In the two-pole approximation they are the shifts of the "atomic" levels. In consequence of this the activation energy of hole-doublon pair is renormalized ($U \to U + \epsilon_2 - \epsilon_1$). The obtained two-pole spectrum is exact in atomic and band limits, temperature dependent, reproduces the Hartree-Foch spectrum in the regime of weak interactions and the spectrum calculated with use of perturbation theory in the case of strong interactions ($t - J$ model for $n = 1$), describes the metal-insulator transition.

Taking into account the Hubbard center $\leftrightarrow$ Hubbard band transitions beyond the two-pole approximation leads not only to the "atomic" levels shifts, but also to the levels broadening and quasiparticle damping.

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Effect of the thermal vibration on the acceleration of neutral atoms during a surface phase transition

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The paper explores the possibility and criteria for the acceleration of neutral atoms during phase transitions at the crystal surfaces. It continues similar studies performed for bulk crystals.

The acceleration occurs via a sequence of consecutive atomic collisions during which an atom in the metastable state transfers to a new stable position giving its excess energy to the next atom in the row. The chain of collision may occur coherently and involve a significant number of atoms enabling the last atom in the chain to harvest considerable energy.

The paper considers a phase transition in the system of adatoms at the crystal surface with a filling factor of 1/4. The adatoms, weakly interacting with the surface and being attracted to the sites of the square lattice of the substrate and strongly interacting with each other, may form two types of lattices at the surface: a square lattice and a rectangular base centered lattice. The phase transition between the lattices happens with changing the lattice constant of the substrate.

The acceleration of atoms was confirmed by the methods of molecular dynamics. The largest velocity of the accelerated atoms for different temperatures was determined. The energy of the accelerated atoms is of order of several tens of eV exceeding by much the thermal energy. Additionally to the single atom acceleration a regime in which two atoms were accelerated was observed. Different processes that require a considerable activation energy usually unavailable trough thermal excitations may be facilitated by the emergence of such accelerated atoms during phase transitions. The process that belong to this class are the excitation of the high energy electronic levels with the emission in UV or X-ray ranges, stimulation of the nuclear reactions, etc.

Structural phase transitions in cylindrically confined electronic clusters

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The space-dimensional transformations of an electronic structure in mesoscopic cluster systems are investigated in a classical approach. The model of a cluster with a confinement of the electrostatic nature is used. The model confining potential is assumed to originate from the uniform cylindrical charged distribution (positive background) on a finite length scale and can be found by solving the Poisson Eq. Provided the Coulomb interactions between electrons the cluster model becomes a purely electrostatic system. These systems are characterized by the parameters of background and the values of ionic power. In practice, such kind of systems can be fabricated in dielectric or semiconductor devices.

Numerical calculation of equilibrium electron distributions in neutral clusters results in four types of the space-dimensional structure. There exist quite perfect 1D-grid structures in extended clusters [1]. Lowering of a cluster length leads sequentially to $2D_x$-structures ordered in one of longitudinal planes including a cluster x-axis, then to variety of 3D-structures, and at last to $2D_{yz}$-structures in a transverse yz-plane of oblate clusters. All of the space-dimensional structures are performed on the phase diagram. The changes of space-dimensionality in the cases $1D \leftrightarrow 2D_x$ and $3D \leftrightarrow 2D_{yz}$ can be interpreted as the structural phase transitions of the 2-d order. They reflect abrupt changes (freezing or unfreezing) of the values of space parameters (coordinates) responsible for the space-dimensional transformations of a whole structure whereas the dimensional transformation $2D_x \leftrightarrow 3D$ is accompanied by continuous changes of the space parameters. The results obtained are compared with those for extended 2D-systems of charged particles [2].

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Kinetic theory of transport coefficients for dense gaseous mixtures with multistep interaction

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Model potentials of a square well or a multistep function enable to formulate a kinetic theory for real dense gases and fluids in the pair-collision approximation [1,2]. The collision integral describes explicitly pair processes at distances of interparticle attraction and allows to elucidate the role of attraction in transport processes [3] and relaxation [4]. The transport equation for the potential energy density complements the kinetic equation for the one-particle distribution function (d.f.) and is a necessary constituent of the theory.

We generalize this theory for the multistep potential to the case of mixture and search for the normal solution of the corresponding set of kinetic equations. Using the modified Chapman-Enskog method, integral equations for the first-order corrections to the one-particle d.f. are obtained. The correction to the inverse potential-energy quasi-temperature is deduced from the potential-energy density equation. It turns out to be linear in the divergence of the hydrodynamic velocity and is coupled to the bulk-viscosity terms of the corrections to the d.f.'s. The obtained contributions to the stress tensor, heat flux, and mass diffusion fluxes define the bulk and shear viscosity, thermal conductivity, and diffusion coefficients.

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Peculiarities of the quasi-long-range ordered phase in a diluted two-dimensional XY model

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The results of a study of the XY model on a two-dimensional lattice with quenched nonmagnetic impurities will be reported. The research deals with such important effects of the dilution as the quantitative change in the spacial spin-spin correlations in the quasi-long-range ordered (QLRO) phase and the reduction of the critical temperature characterizing transition from the QLRO phase to a disordered phase. The interplay of structural and topological defects (vortices) essential for this model is studied with proper rigor by means of the Villain model.

The most essential results of the work are the following. The decay of the spin-spin correlation function is found to be of a power-law form with an exponent different from that of the pure model and dependent on the concentration of dilution. The interaction energy of non-magnetic impurities and topological defects as a function of their separation found within the Villain model approves the attractive character of the interaction and allows for the analytic estimation of the vortex-on-vacancy pinning energy. The mentioned expression for the interaction energy allows as well for the theoretical description of the critical temperature reduction basing on the Kosterlitz-Thouless vortex-antivortex pairs dissociation model.

Where possible, the presented analytical findings are compared to the Monte Carlo simulation results for the diluted two-dimensional XY systems performed by the authors or borrowed from the available literature sources exhibiting good agreement.

The equation of state three-dimensional Ising-like system

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The equation of state for the 3D Ising-like system in an external field near the phase transition point is obtained. For this investigation it is used the Collective variables method suggested in [1]. The calculations are performed with the employment of non-Gaussian distributions for order parameter fluctuations. The ρ^4-model approximation is employed. We have found the explicit analytic form for the system free energy at $T > T_c$ and $T < T_c$ as sum of contributions from different regimes of order parameter fluctuations. Basing on these expressions generalized equation of state containing the dependence on both temperature and field is derived. It is reduced to the scaling form and compared with results obtained by Monte-Carlo simulations [2]. The qualitative agreement with simulation data is demonstrated.

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Critical behavior of 3D Ising-like systems in an external field

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The development of the generalized theory which could allow one to get (except the calculation of critical exponents and some other universal characteristics) explicit expressions for physical quantities is the actual problem for description of critical phenomena The scaling theory is the most developed in respect to this problem. It is based on the scheme of effective Kadanoff spin blocks constructing [1]. We consider the system based on the Ising model on the simple cubic lattice with lattice constant c. The initial lattice is splitted into blocks with linear sizes $s \cdot c$, where s is an arbitrary number ($s > 1$) [2]. Then instead of N initial sites with period c we get N_1 sites ($N_1 = Ns^{-d}$) with period $c_1 (c_1 = cs)$ every of which contains s^d spins. Near the phase transition point (PTP) the free energy of effective spins F_s is related to the free energy of initial spins F by the known relation $F(\tau, h) = s^{-d} F_s \left(s^{y_t}\tau, s^{y_h} h\right)$, where $\tau = (T - T_c)/T_c$ is reduced temperature, h is external field, y_τ and y_h are some numbers defined by critical exponents $y_t = 1/\nu, \quad y_h = 1/\mu$. Here ν is the critical exponent of the correlation length at an absence of the external field $\xi_\tau = \xi^{\pm} |\tau|^{-\nu}$, and μ is the critical exponent of the same quantity $\xi_h = \xi^{(c)} h^{-\mu}$ at $T = T_c$. It is known that $\mu = \nu/\beta\delta$, where β and δ are critical exponents (temperature and field ones) of the order parameter. In this communications the method for free energy calculation near the second order phase transition point is suggested. The explicit analytical expression for free energy of the Ising-like system as function of the temperature and external field is found. This expression allows one to calculate magnetization, susceptibility, heat capacity and other thermodynamic characteristics near the phase transition point.

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A statistical field theory approach applied to the liquid vapor interface

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During the recent years, there has been a renewed interest in the utilization of statistical field theory methods to the description of systems at equilibrium both in the vicinity and away from critical points, in particular in the field of liquid state physics. These works deal in general with homogeneous systems, although recently the study of liquids in the vicinity of hard walls has been considered in this way. On the other hand, effective hamiltonian pertaining to the ϕ^4 theory family have been written and extensively used for the description of inhomogeneous systems either at the simple interface between equilibrium phases or for the description of wetting. In the present work, we focus on the field theory description of the liquid vapor interface of simple fluids. We start from the representation of the grand partition function obtained from the Hubbard-Stratonovich tranform leading to an exact formulation of the problem, namely neither introducing an effective hamiltonian nor associating the field to the one-body density of the liquid. Using as a reference system the hard sphere fluid and imposing the coexistence condition, the expansion of the hamiltonian obtained yields a usual ϕ^4 theory without unknown parameter. An important point is that the so-called capillary wave theory appears as a natural approximation of the one-loop level in the functional expansion of the hamiltonian, without any reference to the underlying phenomenology. Further possible developments will be discussed.

Lattice dynamical study of phase transitions in TlH_2PO_4 and TlD_2PO_4 crystals

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The contribution presents the results of the lattice dynamical simulation of TlH_2PO_4 and TlD_2PO_4 crystals in different temperature phases. At high temperature TlH_2PO_4 and TlD_2PO_4 crystallize with the same orthorhombic *Pbcn* structure (Z=4). However, TlH_2PO_4 exhibits the transition to ferrodistorsive ferroelastic $P2_111/b$ phase (Z=4), whereas the TlD_2PO_4 demonstrates the antiferroelectric phase transition to $P1121/b$ phase which is accompanied with the unit cell doubling along the *a*-axis (Z=8).

The aim of our study was to explain the microscopic mechanism leading to the phase transitions of different character in TlH_2PO_4 and TlD_2PO_4. The lattice dynamics of these crystals was simulated within the semi-empirical approach assuming the Coulomb, short range Born-Mayer type, covalent and hydrogen bonded interatomic interactions. The phonon dispersion relations, partial density of phonon states, dispersion of atomic mean square displacements and temperature factors were calculated in various structural phases.

As follows from our simulation, the protons placed on the shorter $O-H_1\cdots O$ hydrogen bonds play the crucial role at the para – ferroelastic transition in TlH_2PO_4. The 2 % variation of the interatomic interaction within the $O-H_1\cdots O$ bonds leads to the softening of the lowest frequency B_{3g} optic mode in Γ point. However, the proper ferroelastic phase appears as the result of the bilinear interaction between the soft B_{3g} and B_{1u} acoustic V_{YZ} (C_{44}) mode.

The $O-D_2\cdots O$ longer bonds play more significant role at the para – antiferroelectric phase transition in TlD_2PO_4. The slight variation of the interatomic interaction within the $O-D_2\cdots O$ hydrogen bonds of TlD_2PO_4 results in falling down of the S^{1+} phonon branch in $(1/2, 1/2, 0)$ point and evokes the antiferroelectric phase transition.

Modeling of cationic polyelectrolyte solutions in water: influence of the hydrophobic groups on interaction with sodium halides

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We investigated the electrostatic and hydrophobic effects in aqueous solutions of charged chain–like polyions. An explicit water molecular dynamics simulation results for solutions of aliphatic 3,3 and 6,6 ionene oligocation (six monomer units long) in mixture with various low–molecular weight electrolytes are presented. Fluorine, chlorine, bromine, and iodine anions are chosen as the counterions, and sodium ion is the coion in all cases. Different numbers of methylene groups (three in 3,3 and six in 6,6 ionene) separate charged groups and regulate degree of electrostatic/hydrophobic impact of oligocations on the system properties. The explicit water approach reveals the ion–specific effects important for understanding counterion–polyion association. Due to the smaller charge density of the 6,6 ionene, less counterions are located around the oligoion. We also found that the presence of extra hydrophobic groups on the 6,6 ionene shifts the hydrating waters toward the larger distances in comparison with the corresponding 3,3 ionene molecule. The simulation helps us to understand the behavior of osmotic coefficients observed experimentally in aqueous solutions of ionenes with varying degree of hydrophobicity and different counterions. The study seem to explain low osmotic pressure measured in aqueous solutions of polyelectrolyes containing hydrophobic groups.

Deformational effects in the two-positional lattice gas approach for intercalated systems

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Such widely known cathode of lithium-ion cells as lithium intercalated anatase demonstrates a phase separation into Li-rich and Li-poor phases in the whole range of lithium concentration ($x = 0 - 0.6$) as well as two possible positions for Li ion in the oxygen tetrahedron for both phases. In the Li-rich phase intercalation induces lattice deformation causing the antidistorsive internal field and thus making the Li positions nonequivalent.

Performed here symmetry analysis reveals that the observed $U_{xx} - U_{yy}$ deformation in the ab plane and the ordering of antiferroelectric type along the z axis are both described by the B_{1g} irreducible representation of the initial D_{4h} symmetry group and hence they occur simultaneously (so-called internal piezoeffect). According to the Landau expansion approach a phase transition (or separation) with jump of the concentration can be accompanied by the respective appearance of antipolarization.

Microscopic description of the Li-ion subsystem in anatase is given in the framework of the lattice model combining features of the Blume-Emery-Griffiths and Mitsui models, which takes into account all the abovementioned effects. Analysis of the ground-state phase diagram "external field – chemical potential" establishes values of model parameters providing a phase transition between the empty and half-filled phases with appearance of the ordering of antiferroelectric type for both cases of free and clamped crystal. Respective phase diagrams are built also for non-zero temperatures revealing a complicated structure of phase surfaces and lines of critical points. Thermodynamics of the system is studied for both cases of constant chemical potential and constant lithium concentration (leading to the phase separation onto Li-rich and Li-poor domains). Even at the absence of the total polarization, dielectric and (what seems more important) elastic characteristics of the crystal demonstrate jump-like behaviour in the critical points. Concentrational dependence of the incremental capacity $\mathrm{d}x/\mathrm{d}\mu$ (measured by experiment) is calculated and analysed.

Dynamic properties of the Mitsui model with transverse field. Application to the Rochelle salt crystal

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We study dynamic dielectric response of the Mitsui model with consideration for transverse field. This field occurs due to dynamic flipping of ordering structure elements between two equilibrium positions.

Applying the Mitsui model to Rochelle salt, we additionally take into account piezoelectric interaction with shear strain ε_4. We carried out our study within the Bloch equations method. We derived the expression for dynamic dielectric permittivity, which, generally, consists of six modes. These modes could be of relaxation or resonance type depending on temperature and theory model parameters. In paraelectric phases number of modes reduces to three. Dynamic dielectric permittivity of the Mitsui model without consideration for transverse field consists of only two relaxation modes. Applying the developed approach to Rochelle salt, we used theory model parameters derived earlier under condition of agreement of theory and experiment for thermodynamic characteristics. We derived that only one relaxation mode reveals itself in microwave region in case of Rochelle salt. The contribution of other modes to the dielectric dispersion is negligible in microwave region. Hence the dielectric permittivity is strictly of relaxation (Debye) type as experiment shows.

Increasing frequency leads to redistribution of modes contribution to the dielectric permittivity. So, at $T = 80$K (low temperature paraelectric phase) one resonant mode becomes dominant and sharp peak on the imaginary part of dielectric permittivity at $8{\cdot}10^{12}$Hz appears. Increasing temperature smooths resonant peak. Similar behaviour of dielectric permittivity was observed on experiment. However, experiment shows resonant peak at much more lower frequencies, namely $6.6{\cdot}10^{11}$Hz. Yet we can't explain such discrepancy. We performed a comprehensive research of dynamic permittivity dependence on transverse field. Similarly, we studied dynamic dielectric permittivity of $RbHSO_4$ crystal.

Heterophase states and secondary liquid phase

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Ya.I. Frenkel has developed the theory of non-interacting heterophase fluctuations [1] which was reconsidered by M. Fisher [2] in the droplet model of critical phenomena. The fluctuon model of interacting heterophase fluctuations generalizes Frenkel's model and gives description of the essentially heterophase liquid states [3,4]. As shown in [5], frustration plays a key role at the mode of liquid-to-glass transformation determining the width of glass transition temperature range. In [5] volumetric interaction of fluctuons was ignored. Meanwhile, just this interaction causes correlations of fluctuons, as follows from Bogolyubov's theory.

A fluctuon model of heterophase state, taking into account the frustration and volumetric interactions of heterophase fluctuations, is formulated and used for description of the heterophase liquid states. Within the framework of this model the theory of the fluid solidification is developed. It is found that the width of a temperature band of a glass transition is proportional to the renormalized frustration parameter. The equations for a pair correlation function of fluctuons are deduced and the solutions of these equations are found at the pair volumetric interactions described by Yukawa potential. It is shown that volumetric interaction under special condition cause formation of the fractal aggregates of fluctuons. The fractal dimension is larger than 1 and equal to or less than 3. The correlation length is considerably larger than the range of Yukawa potential. It is shown that the liquid state with the fractal fluctuon aggregations (the Fischer cluster) is a secondary phase. Thermodynamics of the secondary phase is investigated. It occurs that that transformation of the secondary phase into primary one and vice versa is the 1^{st} order phase transition. The relaxation spectrum (ultra slow modes) of the fluctuon pair correlations is determined.

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Gauge field theory approach to spin transport in semi-conductors

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We discuss the Pauli Hamiltonian within a $SU(2)$ gauge theory interpretation, where the gauge symmetry is broken. This interpretation carries directly over to the structural inversion asymmetric spin-orbit interactions in semiconductors and offers new insight into the problem of spin currents in the condensed matter environment. The central results is that symmetry breaking leads to zero spin conductivity in contrast to predictions of Gauge symmetric treatments. Computing the translation operator commutation relations comprising the simplest possible structural inversion asymmetry due to an external electric field, we derive a new condition for orbit quantization. The relation between the topological nature of this effect is consistent with our non-Abelian gauge symmetry breaking scenario.

Quantum kinetic theory of ultrafast relaxation processes

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Excitation and subsequent relaxation of quantum many-body systems is an old topic of statistical physics where fundamental contributions came from N.N. Bogolyubov [1]. During the last 15 years this issue has gained considerable new importance due to the development of femtosecond laser sources of intense optical and UV radiation. Their application to atoms and solids has made it possible to initiate and probe electronic relaxation processes on times of the order of a femtosecond or even below. A consistent theoretical description of these processes require the use of quantum kinetic theories which are applicable to times shorter than the correlation time introduced by Bogolyubov.

We have, in recent years, developed a generalized non-Markovian quantum kinetic theory which fulfills these requirements [2]. I give an overview on the two possible concepts which are based on density operators and nonequilibrium Green's functions, respectively [2,3] and present numerical results for dense plasmas, electrons in quantum dots and the photoionization of atoms by a femtosecond laser pulse.

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Mass-dependence of self-diffusion coefficients in disparate-mass binary fluid mixtures

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Binary fluids with strong asymmetry in masses, sizes or charges of particles, forming a mixture present a good example of the system with complicated multiscale dynamics. As the result of asymmetry special features of such mixtures are revealed: fast sound, anomalous diffusion, dynamic arrest and cage effect, crossover to Brownian limit, etc. Some of these features can be observed already on the behaviour of self-diffusion. In particular, $D_2/D_1 \sim (m_1/m_2)^{\kappa}$, where D_2 and D_1 are the self-diffusion coefficients of heavy and light particles correspondingly, m_2 and m_1 are masses. The coefficient κ is equal to 0.5 in the kinetic theory, it varies from 0.06 to 0.1 according to simulation results, and should be equal to 0 in Brownian limit because of mass independence.

Self-diffusion coefficients were calculated within memory function formalism, using the systematic subsequence of approximations for the relaxation times of velocity autocorrelation function. In the limit $\mu \ll 1$ we obtain:

$$D_i = \frac{k_B T}{\sqrt{m_1}} \cdot A^{(i)}(1 + B_1^{(i)}\mu + B_2^{(i)}\mu^2 + \ldots),$$

where μ is the ratio of masses of light and heavy particles; $A^{(i)}, B_1^{(i)}, B_2^{(i)}$ are some coefficients which are expressed via static correlation functions and do not depend on the masses. The obtained expression has a correct Brownian limit. We developed the hierarchy of approximations for $A^{(i)}, B_1^{(i)}$ and $B_2^{(i)}$ that tends to exact result from above and below when the order of approximations increases. The results are planned to be tested in molecular dynamics.

Mesoscopic theory for soft-matter systems

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Mesoscopic theory for soft-matter systems that combines density functional and statistical field theory is derived by a systematic coarse-graining procedure for particles interacting with spherically-symmetric potentials of arbitrary form. In the special case of weak ordering on the mesoscopic length scale the theory takes the form similar to either the Landau-Ginzburg-Wilson (LGW) or the Landau-Brazovskii (LB) field theory, depending on the form of the (effective) interaction potential between particles. Phenomenological parameters that appear in the Landau-type theories are expressed in terms of thermodynamic variables and parameters characterizing (effective) interactions.

Within the framework of this theory we obtain either separation into uniform phases (LGW case), or formation of soft crystals (LB case). In the latter case the theory predicts universal sequence of phases: disordered, bcc, hexagonal, lamellar, inverted hexagonal, inverted bcc, disordered, for increasing density of particles, well below the close-packing density. The sequence of phases agrees with experimental observations and with simulations of many self-assembling systems. In addition to the above phases, more complex phases may appear depending on the interaction potentials. For a particular form of the short-range attraction long-range repulsion potential we find the bicontinuous gyroid phase (Ia3d symmetry) that may be related to a network forming cluster of colloids in a mixture of colloids and nonadsorbing polymers.

Simple three-state lattice model for water

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A simple three-states lattice model that incorporates two states for locally ordered and disordered forms of liquid water in addition to empty cells is introduced. The model is isomorphic to the Blume-Emery-Griffith model. The locally ordered (O) and disordered (D) forms of water are treated as two components, and we assume that the density of the D component is larger. The density of the sample is determined by the fraction of cells occupied by the O and D forms of water. Due to the larger density of the D state, the strength of the Van der Waals (vdW) interactions of the pairs O-O, O-D, and D-D increases. On the other hand, the H-bond interactions are assumed only for the O-O pairs. For the vdW and H-bond interaction parameters and the density ratio of the close-packed and ice forms of water compatible with experimentally known values we find liquid-vapour and liquid-liquid transitions and the corresponding critical points in good agreement with other approaches. All major water anomalies are correctly predicted within mean-field approximation on a qualitative level.

Field theory for classical systems. Entropic effects. Application to non homogeneous electrolytes

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We consider a field theory approach of the liquid state. The Hamiltonian includes the standard interaction as for particles and a term which takes into account the indistinguishability symmetry property known for particles in terms of fields. This term is essentially entropic and accounts for the combinatorics of the particles. The peculiarity of this framework is that these energetic and entropic properties are treated at equal level when we describe the fluctuations of the fields. Such new formalism leads to new interpretations of different physical problems. The approach is exact [1].

The role of the combinatorics entropy is evidently emphasized in the case of ionic systems where there are at least two distinct species and one has to account for their combinatorics. For an ionic system at a neutral interface, we show the existence of a depletion profile for the total density. This phenomenon gives a simple interpretation of the so-called anomalous behaviour of the electric capacitance with the temperature [2]. Within a basic point ion model, we show that an entropic coupling between the total density and the charge field is important. Expressions are then corrected to include excluded volume effects [3]. The formalism can easily be generalised to asymmetric in valence electrolytes where the ionic number balance is modified in order to satisfy the electroneutrality condition [4]. The simple parametrisation of these systems illustrates the capabilities of the approach.

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Effective forces due to confined nearly critical fluctuations

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When macroscopic bodies are immersed into a medium exhibiting nearly critical fluctuations, long-ranged effective forces between them result. Such fluctuation-induced forces are akin to, though distinct from, the Casimir force between two grounded, perfectly conducting metallic plates caused by their influence on the quantum fluctuations of the electromagnetic field. A survey of current theories of such fluctuation-induced forces is given. Their achievements and limitations are discussed in the light of recent experimental results. The role of boundary conditions, their scale dependence, and the consequences of zero modes are explained along with the universal features of these fluctuation-induced forces and conditions under which they are attractive.

Fluids confined in random porous media: Some recent progresses

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In this talk, we present some recent progresses in the study of fluid adsorption in random porous matrices in two directions. The first concerns the development of some analytical equations of state. Although intense investigations have been made during the last two decades, no analytical result has been found for any non trivial off-lattice model for fluids in random porous media. Recently, we have succeeded in extending the scaled particle theory to a HS fluid confined in some model matrices. The agreement between our SPT and simulation results is fine (errors $\leq 20\%$). An empirical correction to the SPT was found which leads to a highly accurate EOS over the whole density range with errors comparable to the simulation ones.

In the second part of the talk, we will present some results on the study of hard sponge model. The morphology of many porous materials is sponge-like. Despite the abundance of such materials, simple models which allow for theoretical description of these materials have been proposed only recently [1]. Ornstein-Zernike type integral equations have been formulated for this model. The numerical solution of these equations requires closure relations between total and direct correlation functions. Although HNC and PY like closures can be formulated also for the hard sponge model, we will show that these popular closures for bulk fluids have serious flaws for the fluids confined in a hard sponge matrix. Some possible strategies for formulating appropriate closures will be discussed.

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Ground states of lattice gas models on the triangular and honeycomb lattices: devil's step and quasicrystals

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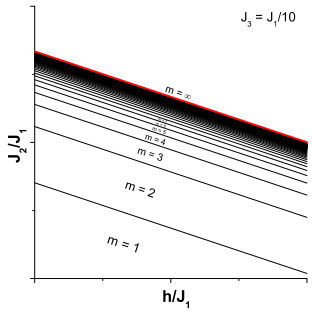
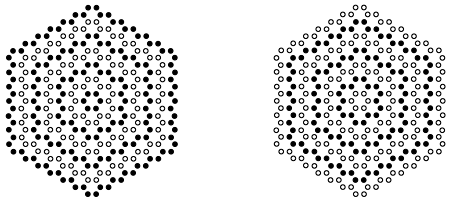
I propose a method for determining the ground states of lattice gas (or Ising) models. The method makes possible to find all types of ground states, including chaotic and ordered-but-aperiodic ones, and to identify the first order phase transitions between them. Using this method, I prove the existence of an infinite series of ground states (the so-called "devil's step") in the lattice gas model on the triangular lattice with up to third nearest-neighbor interactions and I study the effect of the interactions up to 19-th neighbors on this series. To my best knowledge, this is only the second example of the devil's step at zero temperature in the lattice gas models with one kind of particles.





Correlation functions and amplitude ratio for relaxational dynamics with energy conservation

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The dynamic correlation functions for a dynamical model including the nonconserved order parameter coupled to one conserved density (model C) [1] are studied by field-theoretical renormalization group approach [2]. Scaling functions for the characteristic frequencies as well as for the dynamic shape are calculated in one loop approximation. Using an exponentiation procedure these results are extended in order to consider the changes in these function using the fixed point values and exponents in two loop order. The dynamical amplitude ratio R [3] of the characteristic frequencies is generalized to the whole region of wave vector and correlation length. Surprisingly the decay of the shape functions at large scaled frequency does not behave as expected from applying usual scaling arguments. However such behavior for the order parameter correlation function is also found [4] in the dynamics of the antiferromagnet (model G).

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Public transport networks under random failure and directed attack

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The behavior of complex networks under failure or attack depends strongly on the specific scenario. Of special interest are scale-free networks, which are usually seen as robust under random failure but appear to be especially vulnerable to targeted attacks. In a recent study of public transport networks (PTNs) of 14 major cities of the world we have shown that these systems when represented by appropriate graphs may exhibit scale-free behaviour [Physica A 380, 585 (2007)]. Our present analysis focuses on the effects of defunct or removed nodes on the connectivity properties of a PTN. We confirm that the impact of random failure is weak and that for a moderate share of defunct nodes there is little to no change in the network behaviour. Simulating different directed attack strategies however, we derive vulnerability criteria that result in minimal strategies with high impact on these systems.

The correlations between the properties measured for the undisturbed networks and their behavior under attack which we observe are shown to be explained by percolation theory on scale free networks.

Surprisingly we find that the PTNs of cities of similar history and structure may exhibit very different vulnerability levels.

Sound contributions to the short time dynamics of a quasi-1D colloidal suspension

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Description of colloidal dynamics on the level of the Smoluchowski equation assumes the diffusive time limit where other transport processes, such as ballistic motion and velocity relaxation, are coarse-grained. In this description, dynamics of the particles is differentiated into two distinct regimes: the short time dynamics determined by the hydrodynamic interactions, and the long time dynamics within which the configurational relaxation occurs and which is governed by the direct interparticle interactions. The hydrodynamic contributions in the short time regime is characterized by the wave dependent hydrodynamic function, $H(q)$.

In our work we investigate the short time collective dynamics of a colloidal suspension in a quasi-1D channel using the lattice-Boltzmann simulation. The tight confinement of a fluid gives rise to an effective friction in the Navier-Stokes description of a fluid. Consequently, the sound, unimportant in an unbounded fluid, change from a propagating to diffusive behavior, giving rise to an algebraic long time tail in the velocity correlation functions. This prolongation of the sound contributions alters the structure of the hydrodynamic function, $H(q)$, and undermines the assumption in the Smoluchowski description of the clear cut time scale separation. We investigate how the diffusive sound alters the function $H(q)$ and determine the time scale in which it might be observed.

The thermodynamic stability of statistical models in the supercritical region

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The conclusion of variety of critical state manifestations is based on combination of limit properties of subcritical and supercritical states. Such a consideration is carried out on the basis of examination of stability requirements.

The basic stability characteristics of a system are the determinant of stability D and the stability coefficients (the SC's). These quantities are inversely proportional to fluctuations of external parameters of the system. At the continuous transitions D and the SC's pass finite minima, that corresponds to the growth of fluctuations. The locus of these minimum is curve of supercritical transition (the lowered stability curve or quasispinodal). The limit case of these continuous transitions, when fluctuations in the system are at the high and D and the SC's pass zero minima, is the critical state. The critical point is also the limit point of some first-kind transition (the limit point of phase equilibrium curve).

In the paper the exactly solvable models of statistical mechanics are considered. Their equations of quasispinodal are derived and the conditions of its passage into phase equilibrium curve are examined.

Gruneisen parameter behaviour in the critical region of metal cerium

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In [1] the fundamental problem of critical state theory concerning the variety of its manifestatins is solved. It is shown that the type of critical behaviour is determined by stability coefficients (the CS's) $\left(\frac{\partial T}{\partial S}\right)_V = \frac{T}{C_V}$ and $\left(-\frac{\partial P}{\partial V}\right)_S$. As it turned out, the quantity $\left(-\frac{\partial T}{\partial V}\right)_S$, related to the CS's, defines the behaviour of Gruneisen parameter G. G is important characteristic of solid. It is associated with its frequency spectrum and defines the anharmonicity of vibration.

The stability theory enables to connect G with stability coefficients and fluctuations in a system by means of $\left(-\frac{\partial T}{\partial V}\right)_S$. Lemmas by Gibbs establish the relationship between stability coefficients and fluctuations of energy and density. It founds to use G as additional characteristic of phase transition and critical state.

There was performed the computation of G for critical region of phase $\gamma \rightleftarrows \alpha$ transition in metal cerium based on the Rainford-Edwards model [2]. It is shown, that with account taken of vibrational energy of metal crystal lattice in the model G passes explicit minima in critical region.

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Square-well fluids

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The simplest model for a fluid is the many-body system with the square-well interactions. In the limit of infinite range vanishing attraction one can get well-known van der Waals equation of state. This equation predicts critical point and liquid-gas transition. The investigation of critical properties of the system with finite-range interaction is more complicated. For three-dimensional systems the dependence of the critical density and critical temperature were studied using virial expansion truncated to the third order. The analytical results are compared with numerical simulations. It was shown that the temperature dependence of the critical density is non-monotone, this result is confirmed by the exact analytical result for one-dimensional systems. Compressibility maps are analyzed and stability problems are discussed.

Statistical mechanics reached at the point where it can explain elementary processes in life phenomena

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It is a common understanding that the molecular recognition is an essential elementary process for protein to function. The molecular recognition is a thermodynamic process which is characterized by the free energy difference between two states of a host-guest system, bound and unbound. On the other hand, the time to reach the thermodynamic equilibrium depends on the free energy barrier mainly associated with the conformational fluctuation of protein. Therefore, the molecular recognition is a thermodynamic process conjugated with the conformational fluctuation of protein.

We have been developing a new theory for the molecular recognition by protein based on the statistical mechanics of liquids, or the 3D-RISM/RISM theory. The theory has demonstrated its amazing capability of "predicting" the process from the first principle. [1] However, what we have investigated so far is an entirely equilibrium process both in protein conformation and solvation.

Recently, we have started to incorporate the conformational fluctuation of protein into the molecular recognition process in two ways. The first of those is a "static" one in which we just shake the protein conformation to find the local minimum of the free energy surface by the combined 3D-RISM/RISM with conformational sampling algorithms, and to see if one can find the distribution of a guest molecule in the recognition site. One example of such studies will be presented in the talk. [2] The other method is to take the "dynamic" fluctuation of protein conformation into account. The process can be described by hybridized 3D-RISM/RISM with the generalized Langevin dynamics theories. The methodology is currently under construction, and some prospective view of the theory will be presented in the lecture.

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On the description of the quantum surface diffusion: Non-markovian effects vs. jump dynamics

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A description of diffusion processes of light particles adsorbed on metallic surfaces is a topical problem of surface physics and of a high interest both for experimentalists and theorists. Even in the case of a tracer diffusion, the memory effects can be present, if the substrate has no time to relax during the adparticle motion. In our studies we focus on the situation when the memory effects play an important role and can not be excluded from consideration.

We consider surface diffusion of a single particle, which performs site-to-site under-barrier hopping, fulfils intrasite motion between the ground and the first excited states within a quantum well and interacts with surface phonons. We obtain a chain of quantum kinetic equations for one-particle distribution functions and non-equilibrium hopping probabilities. The generalized (time-dependent) diffusion coefficients are derived, and the generic non-Markovian diffusion equation is presented both for an infinite lattice model and in a continuous media limit. In the latter case a one-particle distribution function obeys a Telegrapher's equation that could give us a non-monotonic behaviour of the intermediate distribution function at the large values of a wave vector. In a weak coupling limit, when the energy exchange between the adparticle and the substrate (which plays a role of the thermal bath) is very slow, the relaxation times of the generalized diffusion coefficients exceed an inverse Debye frequency by two orders of magnitude. If the vibrational energy is comparable with temperature, there are also pronounced oscillations of the generalized diffusion coefficients. In our studies we also touch upon the recrossing/multiple crossing phenomena, a problem of the long tails of the generalized diffusion coefficients as well as a possibility of long jumps of the adparticle.

Some semi-phenomenological approaches to description of microcracks formation in solids

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We present some semi-phenomenological models of crack formation in solids. It is shown that microcracks with typical lengths $L < L_{min}$ are being healed due to the thermally activated surface diffusion processes, while at the length $L = L_{max}$, at which a maximum of the total energy of the microcrack $U(\varepsilon, L)$ occurs, there is an instantaneous material destruction. Both lengths are found to have a power law dependence $L_{min} \sim c_{min}\varepsilon^{-\alpha}$, and $L_{max} \sim c_{max}\varepsilon^{-\beta}$, where ε denotes a strain in the vicinity of the microcrack.

We also consider a model with possible penetration of a *guest*-particle inside a defect. Mutual repulsion between *host*- and *guest*-particles leads to appearance of metastable defects in the solid. A stability of such microcracks with respect to temperature fluctuations grows in a certain domain of ε and then decreases. An additional assumption of possible bridge formation between *host*- and *guest*-particles extends this region and enlarges the activation energy of crack formation. The "window" of strains, at which the stable microcracks are being formed, also becomes wider.

Carried out qualitative analysis seems to be quite perspective for further calculations of nucleation and growth times of microcracks as well as distribution of characteristic lengths of the defects.

The site-diluted Ising model

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The Ising model with uncorrelated, quenched random-site or random-bond disorder has been controversial in both two and four dimensions. In these dimensions, the leading exponent α, which characterizes the specific-heat critical behaviour, vanishes and no Harris prediction for the consequences of quenched disorder can be made. In the two-dimensional case, the controversy is between the strong universality hypothesis which maintains that the leading critical exponents remain the same as in the pure case and the weak universality hypothesis, which favours dilution-dependent leading critical exponents. Here the random-site version of the model is subject to a finite-size scaling analysis, paying special attention to the implications for multiplicative logarithmic corrections. The analysis is fully supportive of the scaling relations for logarithmic corrections and of the strong scaling hypothesis in the 2D case. In the four-dimensional case unusual corrections to scaling characterize the model, and the precise nature of these corrections has been debated. Progress made in determining the correct 4D scenario is outlined.

Critical Casimir interaction of ellipsoidal colloids with a planar wall

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Based on renormalization group concepts and explicit mean field calculations we study the universal contribution to the effective force and torque acting on an ellipsoidal colloidal particle which is dissolved in a critical fluid and is close to a homogeneous planar substrate. At the same closest distance between the substrate and the surface of the particle, the ellipsoidal particle prefers an orientation parallel to the substrate and the magnitude of the fluctuation induced force is larger than if the orientation of the particle is perpendicular to the substrate. The sign of the critical torque acting on the ellipsoidal particle depends on the type of boundary conditions for the order parameter at the particle and substrate surfaces, and on the pivot with respect to which the particle rotates.

Dynamics of cooperative lattice-charge (spin) coupled phenomena under far equilibrium condition induced by fs laser light irradiation

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In the dynamical process of the photo-induced phase transition, it has been expected that new exotic phase appears under nonequilibrium condition, so called as a false ground state which can never be achieved in the thermally equilibrium ground state. In this talk, we introduce that such new phase can be really achieved in the molecular based correlated system as a result of transformation of charge order pattern due to competition between electron-electron and electron-lattice interactions.

Here, we mainly discuss about the gigantic photo response observed for the quasi-one-dimensional, quarter-filled $(EDO\text{-}TTF)_2PF_6$ (EDO-TTF = ethylenedioxy-tetrathiafulvalene) crystals. Compared to other quasi-one-dimensional, quarter-filled systems, $(EDO\text{-}TTF)_2PF_6$ is known to have unique features: the phase transition temperature from metal to insulator is anomaly high ($T_c = 280$ K), the charge order in the low temperature phase is (0110), which represents the order of $D^0D^+D^+D^0$ (D = EDO-TTF), and the EDO-TTF ion is largely deformed in the low temperature phase. In addition, ultrafast gigantic reflectivity change within 200 fs has been recently observed by photo-excitation in the low temperature phase and this reflectivity change was assigned to the photoinduced insulator-to-metal phase transition. We show that photoinduced state is never in agreement with any one in thermal equilibrium utilizing ultrafast spectroscopic method and attributed to creation of intrinsic photoinduced state (false ground state) comparing with the time-dependent numerical calculation. Also we found that the coherent reflectivity oscillation becomes incoherent at mid-infrared probe photon energies and showed that the calculation reproduces this phenomenon

These result clearly shows a key role of dynamical structural science for achieving artificial control of the nature of matters utilizing false ground state under non-equilibrium condition.

Partition function zeros of two-dimensional lattice homopolymers

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We study the zeros of the partition function of lattice homopolymers on two-dimensional square lattices. By solving the polynomial resulting from the partition function, we obtain the zeros in the complex temperature plane, called Fisher zeros. The leading zeros tend to approach the real axis as the chain length increases, and the locus of zeros may intersect the real axis in the limit of infinite chain length. The results suggest the collapse transition in the thermodynamic limit.

Magnetic and thermal properties of the Ising-Hubbard diamond chain

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The ground state and thermodynamic properties at low temperature of a spin-1/2 Ising-Hubbard diamond chain are studied. Ising-like spins occupy the nodal vertices on the line of the chain and mobile electrons are placed in the lateral interstitial vertices. The constants of Ising interaction on opposite sides of a diamond unit are supposed to be equal, but can be different on neighboring sides.

Using the decoration-iteration transformation and the transfer-matrix method, the exact calculation of temperature and external field dependencies of the free energy, entropy, specific heat, magnetization, and susceptibility is performed. The competition between the Hubbard repulsion and the hopping integral is examined for the ground state. It is shown that the Hubbard repulsion leads only to decreasing of antiferromagnetic correlations between mobile electrons caused by hopping processes. We also study the manifestation of this competition in the specific heat, magnetization, and susceptibility temperature dependencies and in the low-temperature magnetization processes.

In the large-value limit of the hopping integral and Hubbard repulsion (when the ratio of the squared hopping integral and the Hubbard repulsion is finite) the chain is shown to be equivalent to the Ising-Heisenberg diamond chain with the isotropic Heisenberg interaction between spins of localized electrons.

Brownian dynamics of a self-propelled particle on a substrate

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The overdamped Brownian motion of a self-propelled particle which is driven by a projected internal force is studied using the Langevin equation method. The swimmer under study is restricted to move along a linear channel or in a two-dimensional plane. Its orientation, the direction of the internal force, is either freely diffusing on the the unit sphere or confined to a plane, which is perpendicular to the substrate. For a subset of the cases considered the impact of a uniaxial torque is also investigated. The model is relevant for active particles like catalytically driven Janus particles and bacteria moving on a substrate. Analytical results for the mean position and the mean square displacement are presented and analyzed for several special situations.

The peculiarities of Bose-Einstein condensation of quasiparticles

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The difference between the processes of the Bose-Einstein condensation of particles and quasi-particles is investigated. The equation for the Bose-condensate particle number as a function of the total number of particles in the system is obtained. The same equation is also written for the case of quasi-particles with taking into account their creation by external electromagnetic field – pumping – and the existence of the equilibrium thermal excitations in the system. From the analysis of the both these equations the chemical potential of pumped quasi-particles and their number in the Bose-condensate as a function of pumping intensity is found. It is shown that for low-energy quasi-particle excitations the Bose-Einstein condensation begins and proceeds at arbitrary temperatures, high enough included.

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Investigation of phase diagram of hard-core boson model allowing for non-ergodic contributions

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Recently, a great rising of interest to quantum lattice gas models, particularly to hard-core boson model, is observed. The latter was applied to description of thermodynamics and energy spectrum of system of ultracold atoms in optical lattices and is used also in the theory of ionic conductors and intercalated compounds. In the pseudospin representation one can consider the equivalent XXZ anisotropic Heisenberg model.

Applying diagrammatic technique for Matsubara Green's functions built on pseudospin operators we investigate the contributions on the zero Matsubara frequency, which manifest the non-ergodicity of system and are responsible for difference between isothermal and isolated susceptibilities. The single-particle Green's function and grand canonical potential are calculated in the random phase approximation. Basing on the instability condition in the $\vec{q} = 0$, $\omega = 0$ point, the region of existence of the non-ordered (normal) phase is established. The phase boundary, which corresponds to the second-order phase transition to the phase with the non-zero transverse pseudospin component (phase with the off-diagonal long range order, which is of the Bose condensate phase type) is found. The coexistence lines, describing transitions to the phases with the double modulation of the lattice site occupation and the condensate parameter, are also obtained. Changes in the phase diagram connected with the mentioned above non-ergodic contributions are analysed. A comparison with the results obtained in the decoupling approach for the two-time Zubarev Green's functions is made.

Phase diagrams of Bose-Hubbard model

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The phase transitions in the many-state Bose-Hubbard model are investigated. The interest to this model greatly increased in last years due to the experimental realization of the optical lattices. This model can also be applied for the description of ionic conductivity and intercalation in crystals as well as kinetics of ionic adsorption on the crystal surfaces.

Single-particle Green's function is calculated in random phase approximation (which is an analog of Hubbard-I approximation for the case of fermionic Hubbard model) and the formalism of Hubbard operators is used. Single-particle excitations in the Mott insulator phase are studied (the existence of the energy gap at $\vec{k} = 0$ which vanishes at ctitical point is a feature of this phase, reflecting the localized character of atoms) for the case when the interaction between three nearest bands is taken into account.

The regions of existence of superfluid and Mott insulator phases are established and phase diagrams in the plane (μ, t) (the chemical potential-transfer parameter) are built. The influence of temperature change on this transition is analysed and the phase diagram in the (T, μ) plane is calculated. The role of thermal activation of ion hopping is investigated by taking into account the temperature dependence of transfer parameter. The reconstruction of Mott-insulator lobes due to this effect is analysed.

Quantum cooperative phenomena in photoexcited insulators: Exciton Mott transition and electron-hole pair condensation

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We study theoretically quantum cooperative phenomena in "electron-hole (e-h) systems," which are photoexcited states of solids, composed of electrons in a valence band and positive-charged holes (whose number is identical to that of electrons) in the valence band. In the lower-density regime, an electron and a hole form a quasi-bosonic bound state "exciton," resulting in an insulating exciton gas phase. In the higher-density regime, excitons break to electrons and holes due to the screening and the Pauli blocking, and the metallic "e-h plasma" appears. The transition between these two phases is called the "exciton Mott transition," which is investigated with the dynamical mean-field theory (DMFT) and with the slave-boson mean-field theory for the high-dimensional e-h Hubbard model [1]. In lower temperature, the bosonic exciton gas can be turned into the Bose-Einstein condensed (BEC) phase; on the other hand, the fermionic e-h plasma may be condensed to a superconducting-like state (e-h BCS state). We discuss relation between these two condensates using the self-consistent t-matrix and local approximations [2]. At the Conference, we will mention also lower-dimensional cases, where the biexciton crystallization is expected [3]. We shall also compare the e-h systems with other physical systems, e.g., plasmas, cold atoms, and hadron systems.

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Self-similarity degree of deformed statistical ensembles

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We consider self-similar statistical ensembles with the phase space whose volume is invariant under the deformation that squeezes (expands) the coordinate and expands (squeezes) the momentum. Related probability distribution function is shown to possess a discrete symmetry with respect to manifold action of the Jackson derivative to be a homogeneous function with a self-similarity degree q fixed by the condition of invariance under $(n+1)$-fold action of the dilatation operator related. In slightly deformed phase space, we find the homogeneous function is defined with the linear dependence at $n=0$, whereas the self-similarity degree equals the gold mean at $n=1$, and $q \to n$ in the limit $n \to \infty$. Dilatation of the homogeneous function is shown to decrease the self-similarity degree q at $n>0$.

Coupled order parameter system on a scale-free network

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The behaviour of a system with two coupled order parameters on a scale-free network is investigated. The phenomenological approach [1] is generalized into the case of two order parameters. As a microscopic background we consider an anisotropic spin system on a scale-free network in a mean-field approximation. The system is governed by non-trivial critical exponents, which coincide with ones in the case of a single order parameter system. We consider the appearance of logarithmic corrections to the critical exponents, which follow from the characteristic topology of the scale free network. These corrections appear already in mean field theory contrary to the situation in regular lattices where they are an effect of critical fluctuations. The universal amplitude ratios become non-trivial, the low temperature phase is described by a divergent susceptibility for the continuous symmetry [2].

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To the theory of superfluid with triplet order parameter and conformational degrees of freedom

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Thermodynamics of Fermi-liquid with conformational degrees of freedom is constructed and hydrodynamic equations are derived. Thermodynamical values which described Cooper pair form and connected with conformational degrees are represented in terms of triplet order parameter. Influence of conformation properties on thermodynamical and hydrodynamical properties of liquid are investigated and discussed.

Microscopic theory of electromagnetic pulses slowing in a Bose condensate of alkali-metal atoms

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A physical and mathematical basis for a description of interaction of a condensed Bose gas of alkali-metal atoms with a weak electromagnetic field is developed. The microscopic approach allows to construct a theory that can describe the ultraslow light phenomenon in a gas with Bose-Einstein condensates. Now this phenomenon is known and realized in the experimental conditions. In the framework of the developed microscopic theory we demonstrate new possibilities in the study of the resonance characteristics of the gases consisting of alkali-metal atoms. The proposed approach is based on the Green-function formalism and an approximate formulation of the method of second quantization for quantum many-particle systems in the presence of bound states of particles. We also show that the model of an ideal gas of hydrogenlike atoms can be correctly used for a description of the effects relating to the response of a condensate. In terms of the Green functions we find macroscopic characteristics of a system, such as conductivity, permittivity and magnetic permeability. By the use of these quantities we get the dependencies for the velocity of the pulse propagation and its absorption rate on the microscopic characteristics of a condensed gas. For a Bose-Einstein condensate of alkali-metal atoms we find the conditions when the group velocity of weak electromagnetic waves of both the optical and microwave regions is strongly reduced. We also analyze the Zeeman splitting of the hyperfine levels of alkali-metal atoms and show that the group velocity can strongly depend on the magnetic field intensity. The possibility of controlling the ultraslow light phenomenon in this system by a bias field is discussed.

Kinetics of Bogolyubov Brownian oscillator model and the fluctuation-dissipation theorem

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Kinetics of a system described by Langevin equation

$$\dot{\eta}_a(t) = \sum_b \int_0^t d\tau\, \mu_{ab}(\tau)\eta_b(t-\tau) + f_a(t), \qquad (1)$$

is considered. Here $\mu_{ab}(\tau)$ is a memory kernel, which defines processes in the system including dissipation, $f_a(t)$ are Gaussian random force. Problem of the fluctuation-dissipation theorem (FDT) derivation for equation (1) is discussed. The FDT gives relation between the kernel $\mu_{ab}(\tau)$ and correlation function $\varphi_{ab}(t-t') \equiv \overline{f_a(t)f_b(t')}$ and is proved by us with phenomenological methods. The FDT shows that in the absence of memory effects the correlation function $\varphi_{ab}(t) \sim \delta(t)$. Nevertheless, in some papers one can find opposite assumption.

As an example of a system described by equation (1) we consider model of a one-dimensional harmonic oscillator in equilibrium medium which consists of non-interacting harmonic oscillators. This model is an exact solvable one and was studied by Bogolyubov [1] to give an example of transition of a system to equilibrium. In the framework of this model we study assumptions on which our proof of the FDT is based. In paper [1] Bogolyubov derived a kinetic equation for this model as a strict mathematical fact in the limit of small interaction of the Brownian oscillator with the bath. We proposed a derivation of this kinetic equation based on Bogolyubov functional hypothesis to discuss domain of applicability of this hypothesis. Effective initial conditions for this kinetic equation were studied too. Some statements concerning kinetics of this model were verified by a computer simulation.

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Spatially nonuniform relaxation phenomena in electron-phonon subsystem of a solid

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Non-steady transport phenomena in rarefied electron gas interacting with equilibrium phonon subsystem have been considered. The investigation is based on kinetic equation obtained by us which takes into account the influence of non-homogeneity of the system on electron-phonon collisions. The developed theory is close related to polaron theory developed by Bogolyubov [1]. In spatially uniform state of the considered system there are two relaxation processes: attenuation of electron gas velocity $v_l(t)$ and relaxation of electron gas temperature $T(t)$ to phonon gas temperature T_0. The case, in which estimations $T(t)-T_0 \sim \lambda$, $v_l(t) \sim \lambda$(λ is small parameter) are true, we considered in detail. It is shown that leading contribution to nonequilibrium electron distribution function $f_p(T(t), v(t))$ is represented by Maxwell distribution $f_p^M(T(t), v(t))$ incorrect even in the linear approximation in λ:

$$f_p(T, v) = f_p^M(T_0, 0) + A_{p\,l} v_l + B_p(T - T_0) + O(\lambda^2)$$

$$A_{p\,l} \neq \left.\frac{\partial f_p^M(T, v)}{\partial v_l}\right|_{T=T_0,\, v=0}, \qquad B_p \neq \left.\frac{\partial f_p^M(T, v)}{\partial T}\right|_{T=T_0,\, v=0}.$$

Taking into account this result theory of transport phenomena in the system is constructed. In its framework electron distribution function has structure $f_p(x, T(t), v(t), n(t))$ and is a functional of variables $T(x,t)$, $v_l(x,t)$, $n(x,t)$ ($n(x,t)$ is density of the electron gas). Small parameter of this theory λ is introduced by estimations of the type $v_l \sim \lambda$, $T - T_0 \sim \lambda$, $\partial n/\partial x_n \sim \lambda$, $\partial v_l/\partial x_n \sim \lambda^2$, $\partial T/\partial x_n \sim \lambda^2$. This leads to some modification of usual theory of transport in the system [2].

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Bogolyubov reduced description method in kinetics of quasi-steady-state catalysis

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Catalytic kinetics has been investigated in the framework of the Michaelis-Menten model for enzyme kinetics. In this model [1] in the system there are four components: initial matter (substrate), catalyst, bound state of substrate and catalyst (complex), product (structural modification of the substrate). Kinetics of this model is described with equations:

$$\dot{x} = a(u - z_0)x + bu, \quad \dot{u} = -(ax + b + c)u + axz_0 \tag{1}$$

and conservation laws $z = z_0 - u$, $y = x_0 - x - u$. Here x, z, u, y are concentrations of the corresponding components, x_0, z_0, u_0, y_0 are their initial values, a, b, c are constants of reaction velocities. We study the case in which $x_0 \sim \lambda^0$, $z_0 \sim \lambda^1$, $u_0 = 0$, $y_0 = 0$, where λ is small parameter of the theory. The investigation is based on the Bogolyubov reduced description method (see, for example, [2]). We assume that quasi-steady-state stage of evolution of the system is observed after some transition period (at $t \gg \tau_0$). At this stage concentration of the complex $u(t)$ is a function $u(x(t))$ of concentration of the substrate $x(t)$ and function $u(x)$ does not depend on initial state of the system (the functional hypothesis). Therefore, for times $t \gg \tau_0$ we obtain a closed equation for concentration of the substrate $\dot{x}(t) = L(x(t))$. In this situation one has to use effective initial condition to this equation $\tilde{x}_0$ instead of real one x_0 [2]. Values $u(x), L(x), \tilde{x}_0$ were calculated by us in the perturbation theory. The developed theory was compared in computer simulation with exact one based on equations (1). We observed an excellent agreement of both theories.

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Concept of the local equilibrium and hydrodynamic states of phonons of a solid

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Non-steady transport phenomena in phonon subsystem of an insulator have been considered. The investigation is based on an usual kinetic equation [1] which is studied with the Chapman-Enskog method generalized according to Bogolyubov functional hypothesis. At phonon collisions their energy is conserved but their momentum is not conserved. We discuss transport of energy and momentum. In spatially uniform state of the system attenuation of its drift velocity v_l is observed. A case of small velocity v_l was considered in detail. It is shown that leading contribution to nonequilibrium phonon distribution function $f_k(v(t))$ is represented by Plank distribution with velocity $n_k(v(t))$ incorrect even in the linear approximation in velocity:

$$f_k(v) = n_k(T,0) + A_l(k)v_l + O(v^2), \quad A_l(k) \neq \left.\frac{\partial n_k(T,v)}{\partial v_l}\right|_{v=0} \tag{1}$$

$(n_k(T,v) = (e^{\hbar\beta(\omega_k - k_l v_l)} - 1)^{-1}, \beta \equiv T^{-1})$. The drift velocity is defined in this consideration with usual formula

$$\int d^3k f_k(v)k_l = \int d^3k n_k(v)k)_l. \tag{2}$$

So, this definition is a conventional one because the Plank distribution $n_k(v(t))$ is not a correct leading contribution. Taking into account this result theory of transport phenomena in the system (phonon hydrodynamics) is constructed. In its framework phonon distribution function has structure $f_k(x, T(t), v(t))$ and is a functional of variables $T(x,t)$, $v_l(x,t)$. Small parameter of such a theory λ is introduced by estimations of the type $v_l \sim \lambda$, $\partial T/\partial x_n \sim \lambda$, $\partial v_l/\partial x_n \sim \lambda^2$, $\partial^2 T/\partial x_n \partial x_m \sim \lambda^2$.

Analogously Bogolyubov polaron model has been investigated too.

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Generalized Gross-Pitaevskii equation in kinetics of spatially nonuniform Bose condensate

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An approach to kinetics of Bose gas in the presence of condensate developed in paper [1] was simplified and justified by us. We describe state of the system with amplitude $\eta(x,t)$ of wave function of the condensate $\psi(x,t)$ (average value of Bose field operator), velocity of the condensate $v_n(x,t)$ and distribution function of the Bogolyubov quasiparticles $f_p(x,t)$. For these values and for phase $\varphi(x,t)$ ($\psi = \eta e^{i\varphi}$) of the condensate wave function evolution equations were obtained ($v_n = \frac{\hbar}{m}\frac{\partial\varphi}{\partial x_n}$, m is mass of a particle). Small parameter λ of interaction $\Phi(r)$ is chosen in accordance with relations $\Phi(r) \sim \lambda^2, \eta \sim \lambda^{-1}$; gradients of values η, v_n, f_p are considered as small values of the order g. According to our definition a generalized Gross-Pitaevskii equation can be obtained from the derived equations as an equation for ψ or for η and φ in the absence of quasiparticles (i.e. at $f_p = 0$). Let us give here the obtained equations assuming for simplicity that $g \sim \lambda$ and omitting contributions of the order λ^3

$$\dot{\eta} = -v_l\frac{\partial\eta}{\partial x_l} + \{\frac{1}{2\eta}(\frac{\eta}{2}\frac{\partial}{\partial\eta} - 1)n_0(\eta) - \frac{\eta}{2}\}\frac{\partial v_l}{\partial x_l}$$

$$\hbar\dot{\varphi} = -m\mu_0(\eta) - \frac{mv^2}{2} + \frac{\hbar^2\triangle\eta}{2m\eta} - \alpha\frac{\partial}{\partial x_l}(\eta\frac{\partial\eta}{\partial x_l}), \qquad (1)$$

where $n_0(\eta)$, $\mu_0(\eta)$ are equilibrium density of particle number and chemical potential at zero temperature; $\alpha = 4\pi\int drr^4\Phi(r)/3$. Equations (1) was applied by us to studying of wave close to equilibrium and structure of vortexes in the condensate.

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Thermodynamics and relaxation properties of $Rb_{1-x}(NH_4)_xH_2PO_4$ type proton glasses

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We propose a cluster approach for investigation of thermodynamics and relaxation properties (Glauber dynamics) of proton glasses. Within the two-particle cluster approximation and in the framework of the replica symmetric approach we study a simple proton glass model with essential competing short-range and weak long-range interactions for hypercubic lattices. It is shown that the imaginary part of the susceptibility exhibits a low-temperature peak which corresponds to the system transition to a non-ergodic state. The phase diagram for different interaction parameters and random internal field is plotted. We propose a pseudospin model for proton glasses of the $Rb_{1-x}(NH_4)_xH_2PO_4$ type, which takes into account the energy levels of hydrogens (deuterons) around the PO_4 group, long-range interactions between the hydrogen bonds, and an internal random deformational field. We derive a system of equations for the state parameters for the regions which are in the ferroelectric and antiferroelectric states, as well as in the proton glass state. We obtain a qualitative description of the temperature behavior of Edwards-Anderson parameter and dielectric permittivities of $Rb_{1-x}(NH_4)_xH_2PO_4$, $Rb_{1-x}(ND_4)_xD_2PO_4$, $K_{1-x}(NH_4)_xH_2PO_4$, $Rb_{1-x}(NH_4)_xH_2AsO_4$ compounds. Origin of the low-temperature peak in the imaginary part of the dielectric permittivity in the proton glasses is discussed.

A toy model simulations for passivation on metallic surfaces based on stochastic cellular automata

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Passivity of metals has been widely investigated for more than 150 years. Passivity is the reason for metastability of most metallic materials otherwise extremely unstable in usual conditions. The paradox of passivity is that the metal resists corrosion better in more reactive environment. Here we describe a simple approach to account for and explain this paradox. The complicated kinetic models of passive layer in the literature describe an existing passive layer in a quasi 1-dimensional fashion. In contrast, we get information on its roughness and different regimes of morphology and functioning using a discrete lattice discrete time approach of stochastic cellular automata. We use 2-D lattice and assume that the surface metal sites in contact with environment disappear with a probability P_{cor} during one time step forming a product that can diffuse into the environment. We suppose a monotonous relation of $P_{cor} \propto -\log(V)$ on the anodic polarization describing aggressivity of environment. The diffusion is described by asymmetric exclusion random walk which amounts to a kinetic Ising model. The probability $P_{inter}^{N_{broken}}$ of the random step depends on the net number of bonds broken so that at sufficiently high density the walkers produced form a phase as predicted by the Ising model. To avoid problems with awkward boundary conditions we assume that a single walker surrounded by environment sites a has a finite life time and disappears with a given probability of dissolution P_{die}. With this model we reach steady state conditions and reproduce the qualitative shape of polarization curves. In some range of parameters we find a sharp transition from active to passive state marked by a maximum on the polarization curve. We describe the morphological changes of the passive layer induced by polarization.

Spectral densities of one-dimensional Pauli conductor obtained via exact diagonalization technique

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The systems with proton (ionic) conductivity are a subject of many experimental and theoretical studies in recent years. The special attention is paid to superionic (superprotonic) conductors that exhibit transitions to high-temperature superionic phases that are accompanied the redistribution of protons in plains or chains of ionic groups connected by hydrogen bonds. We investigate the energy spectrum of one-dimensional ionic and protonic conductors described by Pauli statistics taking into account ion (proton) transfer as well as the short-range non-local correlation between particles. Both commutator and anticomutator Green's functions constructed of Pauli creation and annihilation operators are calculated using exact diagonalization technique on the basis of states of finite ionic (protonic) chains with periodic boundary conditions. The frequency and temperature dependences of one-particle density of states is calculated. The possibility of metal-insulator like transition with change of temperature is discussed. In the limit of vanishing correlation strength the results are compared with the ones obtained with fermionization procedure [1] while for different correlation strengths the results are compared with the ones obtained with exact diagonalization technique for similar systems described with Fermi statistics [2].

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Dynamical conductivity of the hydrogen bonded structures in charge ordered phases

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The investigation of the charge transfer in system with hydrogen bonds is performed on the bases of proposed pseudospin-electron model [1,2]. The Hamiltonian of the model includes terms which describe the tunneling hopping of protons, electron transfer, the influence of external longitudinal field, electron-proton interaction and direct interaction between protons. Anharmonicity of the displacement of protons is described by the pseudospin formalism. Only two lowest vibrational states in the anharmonic potential well are taken into account ($s = 1/2$).

The possibility of the first- or the second order transitions from uniform phase into phase with doubled lattice period in quasi-one-dimensional structures with hydrogen bonds is studied in framework of proposed pseudospin-electron model. The phase transition lines from the uniform phase into charge ordered phase is determined. The frequency dependence of dynamical conductivity, as well as it changes with temperature and longitudinal field are obtained.

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On two alternative methods in the theory of superconductive contacts

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Two methods of the calculations of the current states in SNS junctions are discussed. The first one uses the Bogolyubov equations which are considered out the spectrum in the complex plane. In the other method the same equations are considered on the spectrum. In both methods we use the quasiclassical equations for description superconductive state. The SN interface may have no electron reflection or in alternative case transmission coeficient D may be less then 1. In the first case we can speak about SNS junction, in the other one – about SINS junction. The SINIS junction was considered too. We show that in the first method the Green functions may be constructed from two solutions: the first is regular on the $+\infty$ and the other is regular on the $-\infty$. Both solutions can be find in quadratures. The second method needs full information about the spectrum. However for the negative part of the spectrum we obtain transcendental equation that can't be solved analytical. Some authors used numerical calculations but we could show that contribution is canceled with the part of contribution of the continual spectrum and we have the result obtained in the first method.

Thermodynamics, geometrical frustration and quantum fluctuations in coupled spin chains

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The linear-perturbation real space renormalization transformation (LPRG) is presented and applied to study quantum spin chains coupled by interchain interaction (k_1) weaker than intrachain one (k). The method is examined in two exact solvable cases: Ising chains on the square and triangular lattices and quantum XY chain. For the Ising model, in the second order in the cumulant epansion, the deviation of the critical temperature from the exact value is less than 1% for $0.5k > k1 > 0.15k$, but even in the case of the standard Ising model ($k_1 = k$) we found the value of T_c which differs by 2% from the exact one. For the quantum XY chain the deviation of the free energy value found by using LPRG from the exact Katsura result is less than 1% for $T/J > 1$, and for rather low temperature $T/J = 0.08$ is about 6%. The LPRG is used to study effects of interchain frustration on the phase transition in 2D Heisenberg spin chains with easy axis along the z direction. It is shown that contrary to the pure Ising model in systems with in-plane interactions (XY), the interchain frustration does not destroy the finite-temperature transition. However, such a frustration changes the character of the phase transition from Ising-like to, probably, Kosterlitz-Thouless-like. We have also applied the LPRG method to calculate the isothermal magnetocaloric coefficient (M_T) for several spin models in disordered phases. Is is demonstrated that in the presence of antiferromagnetic fluctuations, M_T changes sign at some value of the magnetic field. Generally, M_T is negative if magnetic field competes with a short-range order, and consequently it can be an indicator of the change in the short-range correlation.

Multi-fractal behavior of sol-gel transition of anisotropic colloidal particles suspension

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Aggregation and gelation of concentrated colloidal suspensions is a fascinating topic both from a fundamental as well as a technical point of view. In this work, we analyze the dynamical behavior of scattered light intensity of the colloidal Laponite(Si8[Mg5.5 Li0.4 H4.0 O24.0]0.7 Na0.7) nano particles suspension during the Sol-Gel transition by the multi-fractality behavior. Dynamic light scattering(DLS) have been used due to the transparency of suspension and small sized particles to characterize the evolution of the Sol-Gel reaction in terms of the size of the growing gel particles. Using rescaled range analysis (R/S) and extended self-similarity (ESS) on light scattering intensities of Laponite, we described the sol-gel transition during ageing. By increments of the intensity of the light scattering through the liquid like suspension of colloidal particles in the water, we rely on the temporal variation of non-Gaussian parameter as an estimator and criteria of phase transition occurrence in the underlying sample. We find that for far enough from phase transition, the non-Gaussian parameter is almost time independent, while including phase transition, it becomes extremely fluctuated which means unexpected events grow in our system. The Hurst exponent extracted from R/S analysis increased during gelation time and afterward saturated where the system evolutes from ergodic to non-ergodic state (strongly correlated system). Considering the relation between the Hurst exponent and the diffusion coefficient, particle's aggregate as this coefficient decreases by gelation time indicating that the system enters the gel state.

A dilute solution of long-flexible polymer chains trapped between two parallel walls: Massive field theory approach

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The massive field theory approach in fixed space dimensions $d < 4$ is applied to investigate a dilute solution of long-flexible polymer chains in a good solvent trapped between two parallel impenetrable walls. The proposed calculations were performed for all cases of polymer-surface interactions: for two repulsive walls, two inert walls and combination of one repulsive and one inert wall. Taking into account the well known correspondence between the field theoretical ϕ^4 $O(n)$-vector model in the limit $n \to 0$ and the behavior of long-flexible polymer chains in a good solvent allowed to calculate up to one-loop order the monomer density profiles across the slit. Besides, the two-loop order calculations for the critical exponents characterizing the density profiles of end points near the walls were carried out. The obtained results are in good agreement with previous theoretical investigations [1],[2] and with results of Monte Carlo simulations for the case of two repulsive walls [3].

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Massive field theory approach for polymer chains in confined geometries

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Using the massive field theory approach directly at fixed dimensions $d = 3$ we calculated the depletion interaction potential and depletion force between two repulsive, two inert and one repulsive and one inert walls confining a dilute solution of long flexible polymer chains. The obtained calculations for all cases of polymer-surface interactions were performed for the ideal chain and real polymer chain with excluded volume interactions in the wide slit regime. Besides, we used some assumptions which allowed us to estimate the depletion interaction potential in the region of narrow slit. The obtained results are in very good agreement with previous theoretical investigations [1] and with results of Monte Carlo simulations [2] for the case of two repulsive walls. Taking into account Derjaguin approximation we obtained good qualitative agreement with experimental data [3] for the depletion potential between a spherical colloidal particle of big radius and repulsive wall. The obtained results confirm that the depletion interaction potential and the resulting depletion force between two walls are weaker for chains with excluded volume interaction (EVI) than for ideal chains, because the EVI effectively reduces the depletion effect near the walls.

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Computation of universal scaling functions of critical Casimir forces using Monte Carlo simulations

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Effective Casimir forces induced by thermal fluctuations in the vicinity of bulk critical points are studied by means of Monte Carlo simulations. The critical Casimir force in a slab of thickness L scales as $\beta f_{Cas}(T,L) = L^{-d}\theta_{Cas}(L/\xi)$ where $\theta_{Cas}(L/\xi)$ is a universal scaling function and ξ is the bulk correlation length.

A new numerical method based on an integration scheme of free energy differences is used to compute the universal scaling functions of the critical Casimir forces in the critical region. We consider Ising and XY universality classes in 3D systems with film geometries. Several surface universality classes of the confining surfaces are considered, some of which are relevant for recent experiments. The results are compared with corresponding experimental data for wetting films of fluids as well as with other available theoretical results.

Quantum spin-1/2 XX model on a distorted diamond chain and Jordan-Wigner fermionization

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We consider magnetic properties of the quantum spin-1/2 XX model on a distorted diamond chain. The investigated system represents the model with frustrating interaction and may be related to several magnetic compounds such as azurite. We perform the Jordan-Wigner transformation to get the model in terms of spinless fermions. In contrast to the simple spin-1/2 XX chain with the nearest-neighbor interaction, some XX couplings are mapped to four-fermion terms which introduce the fermion interaction into the model. The interaction terms are considered perturbatively within the Hartree-Fock approximation. Using this method, we calculate the ground state and thermodynamic functions of the model and compare results with the available exact ones for some particular cases as well as with the results of numerical approaches.

Modulation of the neutron field in the multiplying condensed matter and coolant

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A problem of the excitation of thermal neutrons density oscillations, of their propagation and spatial damping (or growth) in a multiplying medium with a coolant is studied. A self-consistent system of equations, describing the processes of neutrons density modulation, is formulated. It includes equations of thermal neutron di.usion together with neutron multiplication and capture, as well as the equations of hydro-dynamics of viscous fluid. The heat emission due to nuclear fission is accounted for in the equation of thermal balance. The corresponding entropy production takes place, so the processes in the system are non-adiabatic. The damping of acoustic, neutron and thermal branches of oscillations are found in this neutron multiplying medium with coolant. A dispersion function and complex wave numbers, which determine the particularities of the neutron field modulation, are also obtained. All three branches give additive contribution to the neutron density oscillations. However, their wave numbers and coefficients of spatial damping (at the same frequency) differ greatly from the sound with its high phase velocity and small attenuation to the neutron wave with the damping length, which is comparable with its wavelength. A spatial growth of temperature oscillations is found in the case of large neutron diffusion and weak coupling of neutron density and temperature oscillations. This fact is of importance for the noise diagnostics of the multiplying medium with coolant. Estimations of the neutron field modulation by the different oscillation branches are made. The modulation amplitudes in the neutron and temperature channels are found to be considerably greater than in the acoustical channel. The results of the work can be applied to the development of the methods of noise diagnostics of the incore reactor equipment.

A polydisperse hard spheres model for interatomic correlations in multicomponent metallic melts

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Since the ions behave as a classical liquid in metallic melts, the influence of different contributions of the interionic pair potential to the structure and properties of such systems is considered next way: it is now generally accepted that the structure of simple liquids, at least at high density, is largely determined by geometric factors associated with the packing of the particles caused by strong short-range interionic repulsion and, in contrast, the long-range attractive interactions may, in a first approximation, be regarded as giving rise to a uniform background potential, that provides the cohesive energy of the liquid, but has little effects on its structure formation. So, ion-ion repulsion in a liquid metal may be regarded as the principal factor determining the ionic arrangement and interionic correlations consequently.

Now we propose another way of constructing correlation functions (SF, PCF) of liquid metal using exact HS solutions of OZ, but PCF would keep its natural smoothness at short-range distances. So, in this work, we regard metallic melt as fluid in which the size of particles is characterized by some random HS diameter distributed by a continuous function, that may also be interpreted as a probability density function of sizes. The other properties (like mass, charge etc.) of particles are constant and associated to the geometric center of such particles. Such a model is based on presentation of metallic system as a polydisperse hard sphere mixture and real interatomic interactions are included implicitly and may be regarded as effective macroscopic forces, that transform HS fluid to soft-core one.

The ultimate results show us an increasing of the isothermal compressibility and decreasing of height of the first maximum of the SF of the model fluid vs. a simple HS approximation. Simultaneously we achieved the smooth PCF instead of a sharp one for HS.

Next-neighbour interactions in BCSOS surface model

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In present work was considered further than nearest interaction in BCSOS surface model. Transfer-matrix approach was utilized to supersede studying of BCSOS thermodynamic properties by investigation of appropriate one-dimensional quantum model ground state. All calculations was performed in one-flip approach that corresponds to low temperature regime.

BCSOS model with the nearest neighbour interactions can be mapped to spin-$\frac{1}{2}$ anisotropic Heisenberg chain. By neglecting the non-commutativity of cofactors in transfer-matrix was shown that more distant interactions leads to arising of new terms proportional to $s_j^z s_{j+k}^z$ in the spin Hamiltonian.

Calculation with taking into account the non-commutativity in transfer-matrix was also performed. The transfer-matrix was constructed in form $\mathrm{e}^{\hat{X}}\mathrm{e}^{t\hat{Y}}\mathrm{e}^{\hat{X}}$ and rewritten in limit $t \ll 1$ as series of commutators $[\hat{X}, ...[\hat{X}, \hat{Y}]...]$. Explicit representation for commutators allows to sum up series and write down complex Hamiltonian with multi-spin exchange interactions. Shown, that even for just nearest neighbour interactions in quantum Hamiltonian 4-spin exchange interactions exists and should be accounted.

Effective grain interactions and negative friction in dusty plasmas

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The kinetic equations describing plasma particle dynamics in dusty plasma are formulated on the basis of the appropriate Bogolyubov-Born-Green-Kirkwood-Yvon-hierarchy. The obtained equations are used to describe the effective grain potentials with regard to electron and ion absorption by grain, plasma particle collisions with neutral atoms and molecules and the presence of external electric field. The polarization forces acting on the grain in the plasma particle fluxes generated by the external electric field are calculated and the possibility of existence of the negative drag force is shown. The friction force in the case of the moving grain is also studied and the conditions of negative friction are established.

A quantum generalization of equilibrium statistical thermodynamics

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Two versions of a quantum generalization of equilibrium statistical thermodynamics are offered. A generalized model of an external environment of object – quantum-thermo-stat is used. A thermal equilibrium is characterized by the effective temperature having nonzero restriction from below. This value takes into account joint stochastic influence of quantum and thermal types. Within the macro-version of the theory quantum effects are taken into account directly without using of an operator formalism. Effective macroparameters are entered but traditional ratios between them are kept. Essentially a new macro-parameter of the theory is effective entropy. At low temperatures it comes nearer to the nonzero value equal to Boltzmann constant. Within the micro-version of the theory similar results for macro-parameters of quantum oscillator in thermostat can be received by dint of averaging of micro-parameters on a complex wave function, dependent on temperature. As an essentially new micro-parameter of the theory is determined operator of stochastic influence. The module of the operator average value has a sense of a new macro- parameter – the effective influence. At low temperatures it comes nearer to half of the Planck constant. At any temperatures through the same macro-parameter it is possible to express effective temperature and effective entropy that provides a mutual coordination between the macro- and the micro-versions of the suggested theory. The consent of results between the given theory and experimental data is shown: at the limit of low temperatures the ratio "effective influence to effective entropy" is determined by the ratio of the constants of Planck and Boltzmann. It differs from zero result predicted by the standard statistical mechanics.

Bose-Hubbard model in bosonic dynamical mean-field theory

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We investigate the Bose-Hubbard model within the recently developed bosonic dynamical mean field theory (B-DMFT). To clarify the difference between B-DMFT and the random phase approximation (RPA) we restrict our investigation by normal phases. To solve the single-site problem we use two analytic approaches that are compared. The first technique is based on the different-time decoupling of irreducible parts in the equation of motion approach. In the second approach the perturbation series expansion is used for single site Green's function with diagram technique. As a result of summing up the series the alloy-analogy approximation with higher corrections is obtained. The result is analyzed in the strong coupling limit. In this case, it is shown that for integer particle concentrations the alloy-analogy approximation gives the same criterium for appearing Bose-Einstein condensation as RPA.

The EPR results and interpretation of thermodynamic functions behaviour for SASD type crystals

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Basing on the EPR study and analyses of thermodynamic functions for modified two-sublattice Mitsui-type model in a wide temperature range we try to do the description of the experimentally observed anomalies which take place in SASD crystals family. The two isomorphic crystals $NaNH_4SO_4 \cdot 2H_2O$ and $NaNH_4SeO_4 \cdot 2H_2O$ differ not only in the phase transition temperatures (twice bigger in the second one), but in the type of phase transition order (the second order for the first one and the first order for the second one). All observed experimentally anomalies in dielectric susceptibility, entropy, heat capacity, lattice dynamics behaviour have been consistently studied. The change of the phase transition order has been found depending on the relative contributions of short and long range interactions between particles. In our opinion this situation is characteristic for the investigated crystals.

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Kinetics of electromagnetic field in nonequilibrium medium of emitters

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This work is a generalization of previous investigations of two-level emitters kinetics with the purpose to consider electromagnetic field as a nonequilibrium subsystem. Emitters of the system are considered as located in space identical particles with dipole moments and can be in excited state with energy $\hbar\omega$. Hamilton operator of the system we take in the Dicke quasi-spin formalism

$$\hat{H} = \hbar\omega \sum_a \hat{r}_{az} + \sum_k \hbar\omega_k c^+_{k\alpha} c_{k\alpha} + \frac{\omega}{c} \int d^3x \hat{P}_l(x) \hat{A}_l(x)$$

(see, for example, [1]). Here $\hat{P}_l(x) = 2\sum_a d_{al}\, \hat{r}_{ax} \delta(x - x_a)$ is density of dipole moment of emitters, $\hat{r}_{al}$ is quasi-spin operator, $\hat{A}_l(x)$ is operator of vector potential of electromagnetic field in the Coulomb gauge. So, we neglect by direct emitter-emitter interaction. Our consideration is based on the Bogolyubov reduced description method. As reduced description parameters (RDP) we took average electric and magnetic fields, their binary correlations : $E_l(x,t), B_l(x,t)$, $(E^x_l E^{x'}_n)_t$, $(E^x_l B^{x'}_n)_t$, $(B^x_l B^{x'}_n)_t$ (variables γ_α) and energy density of emitters $\varepsilon(x,t)$ (its operator $\hat{\varepsilon}(x) = \hbar\omega \sum_a \hat{r}_{az} \delta(x - x_a)$). Quasi-equilibrium statistical operator (QESO) of the system was taken in the form $\rho_q = \rho_f(\gamma)\rho_m(\varepsilon) w_d w(\omega)$, where $\rho_f(\gamma)$ is QESO of the field, $\rho_m(\varepsilon) w_d$ is QESO of the emitters (w_d is distribution emitters in space and dipole directions). Also we included in ρ_q distribution function of emitters in frequencies $w(\omega) = [(\omega - \omega_0)^2 + \delta^2]^{-1}\delta/\pi$ to take into account nonresonance interaction of emitters with the field. Therefore, statistical operators of the system must be normalized by formulae a type $\int d\tau d\omega \mathrm{Sp}\rho_q = 1$, where $d\tau$ denotes integration over variables of distribution w_d. As a result evolution equations for RDP have been obtained and analyzed.

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Phase transitions in Ising chains

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An open question in the study of the spin-1/2 Ising model is the solution of the two-dimensional case in the presence of a magnetic field. A possible answer is based on the study of N-coupled linear chains in the limit of large N. Results reported in the literature show that a dimensional crossover from the one to the two dimensional model does not exist. However, what happens if one considers open boundary conditions (BC)? In this talk I show that, for an appropriate choice of the BC, a system of N-chains exhibits a ferromagnetic order characterized by a critical temperature which tends to the Onsager's one as N increases. It is then possible to study the phase diagram in the (T, h) plane and obtain a solution for finite magnetic field.

Spatially confined fluid with the Yukawa potential of interaction

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Hard wall confined fluid with Yukawa potential of interaction is considered. The solution of the inhomogeneous Ornstein-Zernike equation for the pair correlation function is obtained. The expression for the particle density profile is found by the method of functional differentiation of free energy with respect to the external field. The contribution to the behavior of particle density near the surface is made by the initial potential as well as by the collective screening interaction effects. It is shown that the contact value of the profile satisfies the condition of the contact theorem. Dependence of the adsorbtion coefficient on the particle density is calculated. It is also shown that in the case of attractive Yukava interaction the sign of the adsorbtion coefficient changes with the increase of the particle density.

Generalized collective modes in binary metallic glasses

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We report an extension of the approach of Generalized Collective Modes (GCM), which is one of the most advanced methods of analysis of collective dynamics in liquids, on the case of glass systems. The extension permits to treat ultra-slow dynamic variables on the same footing as the hydrodynamic variables and more short-time dynamic variables.

The developed approach is applied to analysis of collective dynamics in a binary metallic glass $Mg_{70}Zn_{30}$. Time correlation functions, derived in molecular dynamics simulations, are analyzed in order to estimate the spectra of longitudinal and transverse collective modes. Special attention is paid to contributions from concentration fluctuations to the Boson-peak modes.

Molecular dynamics simulations of polymer liquid crystals

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Recent developments in computing facilities (especially availability of affordable workstation clusters) enable to focus attention on a new kind of problems that were impossible to simulate a decade ago. One of such examples are various effects that take place in polymeric liquid crystals. These systems combine the features of both the polymer and liquid crystal, enable fine-tuning on the stage of synthesis and found a numerous practical applications (high strength plastics, displays, optical data storage).

We present some recent developments in molecular dynamics simulations of such systems. *Liquid crystalline dendrimer* is studied in isotropic, nematic and smectic A solvent and we concentrate on orientational relaxation of the macromolecule and its equilibrium shape depending on the phase of the solvent and the way the terminal mesogens are attached to the dendritic core. The results are discussed in terms of the connection between molecular shape and its bulk phase.

The second problem addresses the origin of photo-induced deformations in *azobenzene-containing polymer films*. We reproduced the opposite sign of the deformations under uniform linearly polarized light in liquid crystalline and amorphous films, respectively. The simulations revealed underlying microscopic mechanisms of these deformations depending on the details of molecular architecture.

The third problem is the memory effects in *liquid crystalline elastomers* that are potentially attractive for the application as artificial muscles. In our molecular dynamics simulations we reproduce the reversibility of the shape of lightly crosslinked melt of polymer liquid crystal when driven via the smectic–isotropic transition.

The examples presented demonstrate the potential of molecular dynamics simulations in clarification of the microscopic mechanism behind various effects and are a starting point for simulation driven predictions of the properties of new materials.

On the theory of bulk properties of ionic liquid crystals

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The transportation of charges and ions in liquid crystals has attracted much attention recently because these materials are expected to serve as anisotropic conductors due to their self-organized structures. For this purpose the design and control of molecular interactions and microphase-segregated structures in liquid crystals is essential. While various types of ionic liquid crystals have been prepared and investigated experimentally, theories that can explain the influence of the charge distribution on the mesophase stability on ionic liquid crystals are still lacking.

Here we use the density functional theory and a molecular field theory to provide some theoretical insight into the mechanism responsible for the formation of bulk phases in ionic liquid crystals. In particular, we study the dependence of the topology of the phase diagrams on various parameters such as shape, size, charge of the molecules and the temperature.

Phase transitions and quantum stabilization in quantum anharmonic crystals

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A unified theory of phase transitions and quantum effects in quantum anharmonic crystals is presented. The theory is based on the representation of the Gibbs states of the model in terms of path measures. It covers the case of crystals without translation invariance, as well as the case of asymmetric anharmonic potentials. In the simplest case where the lattice is $\mathbf{Z}^d$, the model is translation invariant, and the interaction is of nearest neighbor type with strength $J > 0$, it is found that the key parameter is $8dmJ\vartheta^2$. Herein, m is the particle mass and $\vartheta > 0$ is an anharmonicity parameter. It is proven that the crystal is stable (no phase transitions at all temperatures) whenever $8dmJ\vartheta^2 < 1$. At the same time, a sufficient condition for a phase transition to occur is $8dmJ\vartheta^2 > \phi(d)$, $d \geq 3$, where $\phi(d)$ is an explicitly given function, such that $\phi(d) \to 1$ as $d \to +\infty$.

Method of intermediate problems in the Fröhlich polaron model

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Method of intermediate problems in the theory of semi-bounded operators in rigged Hilbert space was applied to investigation of the ground state energy of the Fröhlich polaron model. It was shown that various infinite sequences of non-decreasing improvable lower bound estimates for the polaron ground state energy can be derived for arbitrary values of the electron-phonon interaction constant. The proposed approach allows for explicit numerical evaluation of the thus obtained lower bound estimates at all orders and can be straightforwardly generalized for investigation of the low-lying branch of the polaron excitation energy spectral curve adjacent to the ground state energy of the polaron at rest. In conjunction with numerous, already derived by multitudinous methods, well-known upper bound estimates for the energy spectral curve of the Fröhlich polaron as a function of the electron-phonon interaction constant and the polaron total momentum, the aforesaid improvable lower bound estimates may provide one with virtually precise magnitude for the energy of the slow-moving polaron.

Theory and atomistic modeling and simulation of relaxation processes in condensed matter

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In this report I will consider the relaxation processes at extreme states that accompany the material response on high rate energy deposition: plastic deformation and fracture of solids and rupture of liquids under high strain rates during shock-wave loading, bulk and surface melting at high pressures and temperatures, effects of ultrafast energy deposition into the electron subsystem on stability of crystals. The level of computational complexity of classical and quantum atomistic models under consideration requires the deployment of the modern supercomputer of the teraflops power. The multiscale approaches are developed for the application of the results on the time and length scales beyond the current direct accessibility of the atomistic methods.

Toward a Hamiltonian evolution dynamics – or why complex dynamical systems crash from time to time

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What are the explanations of natural science in view of systemic meltdowns such as the financial markets and possibly the economic system? Surprisingly little. Systems like the economy, financial markets or the biosphere evolve according to a set of so-called evolution equations, which have been studied or almost a century. Since economy or biology involve millions of goods and services, and species respectively, these equations become practically useless for understanding systemic characteristics of these systems, such as their robustness under shocks, their potential for being self-diversifying, or recovery rates after shocks. We suggest a Hamiltonian interpretation of evolution systems, such that it becomes possible to solve them in terms of their phase structure, especially for extremely high dimensions. These systems exist in two phases, one flourishing, highly diversified phase and a phase of very low diversity, with practically nothing in between. In this framework, the probability for crashes to occur can be directly translated to the 'distance' of the system from the phase transition surface. Our results might provide new ways of thinking about systematic risks and of how to consciously avoid crashes in rational and systematic ways.

Contact theorems for charge and density profiles of ionic fluids on the charged surface

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By the direct integration BBGKY equation between singlet and binary distribution functions of ionic fluid in the presence of charge surface the exact relations (so-called contact theorems) for the contact values of charge and density profiles are obtained [1]. The obtained results are analyzed for symmetrical [2] and nonsymmetrical [3,4] ionic systems. For the electrolytes with a single type of cation and anion, the contact value of charge profiles can be presented as the sum of three contributions. One of them is the normal component of the Maxwell electrostatic stress tensor. The second one is the surface electrostatic property, which is defined as the integral of product of the gradient of the electrical potential and the density distribution function of coions. The third term is the bulk contribution, which is defined by the sum for anions and for cations of the product of their charge and their partial pressure. For noncharged surface, only the last two terms are present and have the same sign in the case of size asymmetry. In the case of charge asymmetry, the contact value of the charge profile is the result of the competitions of bulk and surface terms in which the bulk term is dominant. Using both the contact theorems for the density and the charge profiles, the exact expressions for the contact values of the profiles of coions and counterions are obtained and some related properties are discussed. A semiempirical expression of the contact value of the charge profile is discussed in relation to exact result. Within a field theoretical description, the phenomenon of spontaneous polarization of a neutral hard planar interface for valence asymmetric ionic fluids is discussed. The theoretical results are compared with numerical simulations data and are shown to be in very good agreement.

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Scaled particle theory for one- and two-dimensional hard sphere fluids confined in random porous media

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Scaled particle theory (SPT) is the simple semi-intuitive approach developed 50 years ago for the description of thermodynamical properties of hard sphere fluids [1]. This approach is based on the combination of the exact treatment of point scaled particle in hard sphere fluid with the thermodynamical consideration of finite size scaled particle. Recently SPT approach was extended for the description of a hard sphere fluid confined in random porous media [2]. In result the first very accurate analytical results was obtained for hard sphere fluid in hard-sphere and overlapping hard-sphere matrices.

In this report we present the application of SPT theory for the description of one- and two-dimensional hard sphere fluid in different models of porous media, e.g. Madden-Glandt models [3] of hard-sphere and overlapping hard-sphere matrices, model of the hard-sponge model [4] and model of soft-sponge model [5]. The corresponding expressions for the chemical potentials and equation of state are presented and discussed.

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Structural relaxation at interfaces of transition metal oxides

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In complex heterostructures of transition metal oxides, interface phenomena can lead to novel electronic states not observed in the bulk constituents. For several types of oxide heterostructures, we have studied interface discontinuities due to the lattice mismatch with the substrate and the effects of interface polarity. We have found that structural discontinuities induce a new type of a mixed electronic-lattice reconstruction near the interface which include: (1) the modification of lattice constants and local static atomic displacements in the interfacial region, and (2) a reconstruction of the state of the electron subsystem. One of the example of the considered reconstructions is the metal-insulator transition in the heterostructure of $LaAlO_3$ film and $SrTiO_3$ observed upon the increase of the film thickness. Another mixed process known as orbital reconstruction is related to a change in orbital occupations of the transition metals near the interface which can be activated by structural relaxation. A comparison of the results obtained for oxide interfaces with the experimental studies by scanning tunneling spectroscopy shows a key role of the local Coulomb repulsion in the interfacial electronic properties. As a result, the electronic system at the interface of the oxide heterostructure is not a two-dimensional electron gas (2DEG), but can be described as a two-dimensional electron liquid (2DEL), a new interfacial state recently revealed at titanate-lanthanate interfaces. Interfaces in oxides therefore broaden the spectrum of available two dimensional electron systems from the 2DEGs of conventional semiconductors to also include two-dimensional systems with strong electronic correlations.

Transverse dynamics of binary fluids with mass asymmetry

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We consider the influence of the mass asymmetry on the dynamic behaviour of binary fluid. The investigations are performed by combining the molecular dynamic simulations (MD) and general modes approach (GMA). The MD simulations are performed in the microcanonical ensemble for the system consisting of $N = 1000$ particles at temperature $T = 1.0$ and particle density $\rho = 0.75$. A four-variable analytical model based on the transverse components of mass and mass-concentration flows as well as their first derivatives permits us to obtain the spectrum of collective excitations. It contains the branch corresponding to the transverse sound modes and another branch describing propagating the optic-like excitations in the system.

The dependence of collective mode spectra on the mass asymmetry at the wide region of wave vectors and the mass asymmetry ratio is investigated. We show that in the region of intermediate and small wave vector numbers heavy particles are responsible for the transverse sound modes whereas light particles oscillations determine mainly the spectrum of optic-like excitations. It is found that the range with well defined sound excitations in the total momentum spectral function is reduced with increasing of the mass asymmetry ratio.

The behaviour of the lowest relaxation mode which corresponds to the transverse viscosity in the long-wave limit is considered. It is found the agreement of the result for transverse viscosity calculated in GMA and data received via direct MD simulations.

Generalized diffusion coefficients in multicomponent fluids

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The problem of definition for diffusion coefficients in the multicomponent systems as well as their representation in different reference frames is considered. We perform analytic study of mutual diffusion coefficients within the frames of generalized modes approach. Using the rigorous mathematical formalism the matrix of generalized diffusion coefficients depended on the wave vector and time are obtained as product of the generalized kinetic coefficients matrix and the matrix of static structure factors. In the hydrodynamic limit corresponding Green-Kubo formulas for diffusion coefficients are derived.

With help of simple matrix transformations it is shown that all mutual diffusion coefficients can be reduced to $\nu(\nu-1)/2$ independent dynamical quantities expressed via the corresponding correlation times. Here ν is the number of species in the mixture. The structure of transformation matrixes are found. This allows us to study in detail the transformations between different reference frames and to derive the correct expression for mutual diffusion coefficients.

In order to give an example our approach is used for the study of conductivity properties in a multicomponent charged particles system. In particular, we derived so-called "universal gold rule" for the ratio of partial conductivities for the model of molten salts.

Generalized transport equations for the "gas-semi-bounded metal" system

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The system of transport equations for the spatially inhomogeneous electron gas of semi-bounded metal by the nonequilibrium statistical operator approach is obtained. This set of equations is consistent with averaged Maxwell's equations for electromagnetic fields and give us a possibility to describe the diffusion and polarization processes for magnetic dipoles adsorbed on the surface of transition metals.

Plasma theory of phonons in a liquid

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Well known, that a sound oscillations are polarized atoms of a liquid. In the case of a system of strongly interacting atoms, like a liquid, electrons of external atomic level (valency) can be considered as Fermi-liquid. But for simplicity, to obtain a characteristic value of velocities, we consider it as degenerated Fermi-gas and in this model all sorts of ions will be considered as ideal gases too. Then we have a plasma model with neutrality $\sum_a eZ_a n_{a0} = 0$ (Z_a is charge). The Maxwell equation for self-consistent longitudinal (potential) electric field is $\partial \mathbf{E}/\partial t = -4\pi \sum_a eZ_a n_a \mathbf{v}_a$. Component velocity $\mathbf{v}_a$ can be expressed through electric field with the help of linearized continuity and Euler equations for every component in adiabatic process. And after Fourier transformations we obtain a dispersion equation $1 = \sum_a \Omega_a^2 / \left(\omega^2 - u_a^2 k^2\right)$, where $\Omega_a^2 = 4\pi e^2 Z_a^2 n_{a0}/m_a$ is a square plasma frequency and $u_a^2 = \left(\partial P_a/\partial n_{a0}\right)_s / m_a$, P_a is a component pressure. The dispersion equation gives in general $(a_{max} - 1)$ phonon modes which correspond to every intermediate frequencies $u_a k \ll \omega \ll u_b k$. The largest frequency between electronic and ionic velocities corresponds to acoustic phonon mode and for $k r_{TFe} \ll 1$ ($r_{TFe} = u_e/\Omega_e$ is Thomas-Fermi radius) gives $\omega = k u_e \sum_i \Omega_i/\Omega_e$, like ion sound. Lets suppose, we have two - light (l) and heavy (h) - ion sorts with the same temperature that, from Vlasov kinetic theory is well known, gives dumping of modes with $k u_l \ll \Omega_l$, but if $u_l/\Omega_l \gg 1/k \gg u_h/\Omega_h$ (between Debye radiuses) then we obtain an optic mode $\omega = \Omega_h$. Lets consider extremely low temperatures and bosonic ions (α-particles - helium II, for example). Then for a condensate part (c) of ions $P_c = 0$ and $u_c = 0$. We suppose that $n_c \ll n_{\alpha-c} \sim n_e/2$, then we obtain not only the first sound with $\omega = k u_e \Omega_{\alpha-c}/\Omega_e$ but also the second sound with $\omega = k u_{\alpha-c} \Omega_c/\Omega_{\alpha-c}$ for $k r_{\alpha-c} \ll 1$ ($r_{\alpha-c} = u_{\alpha-c}/\Omega_{\alpha-c}$ is Bose analogy of r_{TF}). And from Vlasov kinetic theory we know, that condensate part of α-particles does not give Cherenkov damping of sound. If we have a small addition of ^3He, it will absorb the second sound when $u_{^3He} \geq u_{\alpha-c}\Omega_c/\Omega_{\alpha-c}$. This condition gives a critical concentration of ^3He in ideal gas approximation.

Time dispersion in the Bogolyubov reduced description method

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The Bogolyubov reduced description method is widely used to construct time equations for parameters of description of macroscopic systems. In this paper the method of reduced description of the nonequilibrium states is applied for consideration of the electromagnetic field (EMF) in a nonrelativistic thermostat from the charged particles of few sorts. Strength of the electric field and vectorial potential in the Hamilton gauge are selected as parameters of the EMF description, which satisfy the Peletminsky-Yatsenko condition that is had oscillated dependence on time. The main idea of the paper consists in the selection of harmonious oscillations with frequency ω_k characterized a selected process as the main characteristic of the EMF time evolution. For this purpose at construction of perturbation theory the following main EMF hamiltonian is selected: $H_0 = \frac{1}{8\pi}\int d\vec{x}\left(\vec{E}^2(\vec{x}) + \frac{1}{c^2}\int d\vec{x}'\omega^2(\vec{x}-\vec{x}')\,\vec{A}(\vec{x})\,\vec{A}(\vec{x}')\right)$. Proper to the interaction of EMF with a thermostat hamiltonian is considered small. The use in the current following after the second approximations is considered in an electrodynamics as the account of nonlinearity, that will give the high degrees of strength and potential of EMF. But absence of nonequilibrium correlations among the parameters of the EMF description is assumed. Only in this case it is possible to get rid of dependence of current on the magnetic field (or vectorial potential) through equation of bond, that will result in expression of potential in interaction picture only through strength. In agreement with the Peletminsky-Yatsenko condition we search the solution as a plane monochromatic wave. Within the second order an electric current is linear on EMF. First by the Bogolyubov method dispersion equations are found not only for short transversal waves but also for long-wave and low-frequency, both longitudinal and transversal EMF. Permeability, that is expressed through the Green functions, is coincided with obtained from other methods. For nonrelativistic limit it is possible to rewrite the interaction hamiltonian through operators of strength of the field, that gives the type of equations of nonlinear electrodynamics absolutely identical to phenomenological.

An augmented van der Waals theory of strongly interacting fluids

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A novel perturbation method for the structural and thermodynamic properties of the fluids with hard core plus attractive interparticle interaction is reported. The method is based on a new reference system, the short-range attractive Yukawa model of the range parameter $z_0 = 6$ that is free of the vapor-liquid phase transition. We show that the inclusion of a short-range part of the total attractive interaction into a reference system allows a natural extension of the traditional first-order perturbation theory of simple fluids to practically all thermodynamic states. The theory is applied to evaluate the structure factor [1], thermodynamic functions and the liquid-vapor coexistence curve [2] of the Lennard-Jones-like medium range and Coulomb-like long range Yukawa fluids as well as to the Sutherland fluid. Comparison with computer simulation data and the second-order Barker-Henderson perturbation theory is discussed.

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Exact solution of the antiferromagnetic sawtooth chain with Ising and Heisenberg bonds

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The sawtooth chain with pairs of $S = 1/2$ spins interacting with XXZ-interactions placed on each second tooth is considered. All other interaction bonds are taken to be of Ising type. Exact statistical mechanical solution of the model within the direct transfer-matrix technique is obtained. The solution allows one to obtain exact analytic expressions for all thermodynamic functions of the model. The ground state phase diagram and plots of magnetization versus external magnetic field are obtained. In contrast to the case of conventional Heisenberg sawtooth chain with all antiferromagnetic couplings the system under consideration exhibits magnetization plateau not only at $M/M_{sat} = 1/2$ but at $M/M_{sat} = 1/4$ as well for certain region of parameters.

Aging and flow in a colloidal suspension

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Understanding the physical mechanisms governing the interplay between aging dynamics and shear flow is crucial to both elucidating the nature of slow dynamics in soft materials and controlling their complex rheological behavior.

We investigate the evolution of the density autocorrelation function of an aging colloidal suspension subject to a steady shear flow (shear rate γ). The competition between the structural relaxation time and the inverse shear rate gives rise to a complex dynamical behavior that we could quantitatively analyze studying the detailed shape of the particles density autocorrelation function. The sample is an aqueous suspension of Laponite, a highly thixotropic liquid which undergoes structural arrest on a timescale which strongly depends on concentration and ionic strength and that can be as long as few months. We found that the aging dynamics displays two different regimes whose boundary is marked by the condition $\tau\gamma = 1$. As long as the characteristic relaxation time τ is small on the time-scale $1/\gamma$, aging is unaffected by the presence of shear. During aging dynamics slows down, and when τ becomes of the order of $1/\gamma$, the system enters a shear dominated regime where aging is strongly reduced and the structural relaxation time is very sensitive to γ. The intermediate scattering functions, characterizing the slow non-equilibrium dynamics of the sheared sample, are well described assuming an heterogeneous scenario where the complex dynamics results from the superposition of relaxing units each one independently coupled to shear rate.

At the same time we monitor velocity profiles by means of heterodyne dynamic light scattering. Shear localization is observed at the lower rates of shear. An un-sheared gel band coexists with a uniformly sheared fluid band whose relaxation time is fixed by the shear rate.

We also study the aging process after rejuvenation of the sample with an high shear rate. The t_w dependence of τ after rejuvenation is substantially different from that observed in normal aging and follow a power law.

We discuss these results in relation to recent theoretical work and present a simple phenomenological model based on Langevin dynamics which is capable of reproducing many of the observed features.

Kinetic equation for the dynamic system interacting with the phonon field in the case of space inhomogeneity

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A construction of kinetic equation for the dynamic system interacting with the phonon field in the case of space inhomogeneity is considered basing on the methods developed in [1–3].

As shown here, approaches [1,2] could be generalized for the case of space inhomogeneity. An arbitrary operator construction depending on momentum, space variable and other parameter is used for derivation of kinetic relationship. We consider the method for study of the electron-phonon system and exclusion of phonon operators from the appropriate operator constructions. In particular, the interaction of an electron with the phonon field is described by kinetic equation for the polaron in the case of space inhomogeneity. In the limit of the appropriate approximation this equation gives the exact Boltzmann equation for polaron.

As shown also, if the parameter tends to zero, our generalized dynamic system reduces to the well-known case of the homogenous model.

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Anharmonicity of $Sn_2P_2S_6$ ferroelectrics

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The ferroelectrics $Sn_2P_2S_6$ (SPS) represent a wide class of low-symmetry compounds, where the strongly pronounced nonlinear phenomena have two origins: the polarizability of the anion sublattice is much higher than in oxides; the symmetry is lower (monoclinic), allowing effects which are forbidden in the high-symmetry perovskite structures. For this compound the second order phase transitions is observed which is near Lifshitz and tricritical points at the state diagram [1].

A reasonable microscopic model for the SPS ferroelectrics was developed [2] in *ab-initio* effective-Hamiltonian approach. It was found that the strong nonlinear coupling between low-energy soft optic mode and other hard modes lead to a triple-well shape of the potential-energy surface. This nonlinearity could be a reflection of the strong polarizability of Sn^{2+} cations in chalcogenide surrounding. Statistical theory for ferroelectrics based on triple-well anharmonic potential was used and model parameters were estimated [3]. It was found confirmation of the assumption that the phase transition in considered crystals is located in crossover region between order-disorder and displacive type, and very closely to tricritical point. Anisotropy of hypersound velocities of SPS crystals is investigated by Brillouin spectroscopy using different scattering geometries. The dispersion of velocity of the longitudinal sound waves was observed which can be connected with the role of acoustic phonons in soft mixed optic-acoustic modes at transition near the Lifshitz point. The linewidth of quasielastic light scattering has been measured at various temperatures. Thermodynamic and dynamic characteristics of the lattice anharmonicity are compared.

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Tests of conformal field theory predictions for the Yang-Lee singularity

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Using finite-size scaling, we test conformal field theory predictions for the structure constant and excitation spectrum at the Yang-Lee singularity of the 2D Ising model.

Football fever: self-affirmation model for goal distributions

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Analyzing football score data with statistical techniques, we investigate how the highly co-operative nature of the game is reflected in averaged properties such as the probability distributions of scored goals for the home and away teams. It turns out that especially the tails of the distributions are *not* well described by the Poissonian or binomial model assuming uncorrelated random events. Instead, a less basic but good effective description of the data is provided by negative binomial or generalized extreme value distributions. To understand this behavior from first principles, we propose to modify the Bernoulli random process underlying the Poissonian model to include a simple component of *self-affirmation* which describes the data surprisingly well and allows to interpret the observed deviation from Gaussian statistics. The phenomenological distributions used before can be understood as special cases within this framework. We analyzed historical football score data from many leagues in Europe as well as from international tournaments, including data from all past tournaments of the "FIFA World Cup" series, and found the proposed models to be applicable rather universally. In particular, here we analyze the results of the German women's premier football league and consider the two separate German men's premier leagues in the East and West during the cold war times and the unified league after 1990 to see how scoring in football and the component of self-affirmation depend on cultural and political circumstances.

Discussed by Michael Hopkin in Nature News Feature article *Goal Beget Goals*, Nature **441**, 793 (2006).

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The shear elasticity of ice Ih near the melting point

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Melting is a fundamental process in which a crystal undergoes a phase transition from a solid to a melt. Despite its common occurrence, understanding this process still a challenge The existing theories of melting are still far from being complete and raise new questions. Hence, the purpose of the present research is to gain a better understanding understanding of the mechanism of melting transition ice-water.

Our study is concerned with internal-friction measurements made at low frequency (torsion pendulum) on specimens of ice Ih. The experimental data of the shear modulus of ice in a temperature interval $213-273K$ at frequencies of $0,3-2$Hz have been obtained. Essential falling of the shear modulus with temperature growth, since $263K$ is revealed. Observable anomaly is contacted with occurrence of a quasiliquid phase. The amount of quasiliquid phase is calculated.

Nonlocal and many-particle effects in the microscopic metal theory

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In frames of a reference system approach a variant of microscopic theory of normal metals was suggested and developed. With the aim of equal description both localized and collectivized electrons in metal we developed a method of an optimal one-particle basis $\{\phi_\sigma\}$ construction. It is a direct sum of two orthogonal subspaces – ion core electron states wave functions and delocalized functions. On this base we obtained the Hamiltonian of the electron-nuclear model, that assumes a direct calculation of matrix elements. This Hamiltonian is an obvious generalization of the well-known Bogolyubov's Hamiltonian [1] in his polar model of metal and considers all correlation, hybridization and orthogonalization effects.

The effective Hamiltonian of electron-ion model obtained with the help of reduction procedure (a statistical averaging over ion core electron states). Thus all interactions become nonlocal and many-particle as for ions, as electrons. The influence of nonlocal and orthogonal effects investigated on the formation of the electron-ion interactions. This approach is generalized on the case of binary metallic systems.

We developed some methods for the partition function calculation (over electron variables) in the adiabatic approximation for the electron-ion model with nonlocal interactions. As a result – the effective Hamiltonian obtained for a quasi-atoms system with two-, three- and four-particle interactions. The latest is presented in the form of decomposition of nonlocal electron-ion potential powers and $\mathbf{k}$-components of n-particle static correlation functions of the electron liquid model. We established a good convergence of such decompositions for $n = 2, 3, 4$. Thus was used a local field correction function, which we obtained in frames of the microscopic theory. We calculated the lattice constant for the fcc structure which deviates from experimental data not more than 1%, using a minimization procedure for a metallic Li energy.

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The microscopic model of the real degenerated dwarfs with gravity and electrical interactions

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The relativistic parameter x_0 was evaluated using data obtained from the "Hipparcos" mission in frames of the standart Chandrasekhar model. This model considers only the relativistic degenerated electron gas contribution to inner pressure of the system and the gravity interaction continual distributed mases of nuclei. The parameter x_0 determines all star characteristics (mass, radius and the energy are monotonous function of x_0). The same calculations were done for the generalized model with non homogeneous chemical compositions that correspond to helium-hidrogen dwarfs. We found that $0.9 \leq x_0 \leq 1.5$ in central part of dwarfs. This means that the electronic system is near to relativistic degeneration but is not in ultrarelativistic state. In this case the general relativistic theory effects and influence of neutronization aren't important. Therefore the Chandrasekhar model in first approach is good aproximation for real degenerated dwarfs. But this model can't explain variation of x_0 values and observed distribution of dwarfs over radii or mases.

We propose the dwarf model that considers not just gravity, but also electrical interactions. This model corresponds to nonhomogeneous metal model in the microscopic theory. The energy in this model was calculated in frames of the reference system approach with interacting relativistic electron gas model as the basis system. Characteristics of dwarfs as functions of x_0 are calculated using mechanical balance equation. To contrast to the Chandrasekhar model full energy obtained in our approach has nonmonotonous dependence from the parameter x_0. The minimun in this function approximately corresponds to observed maximum of real dwarfs distribution over radii.

The calculation of the strong-coupled electron liquid model characteristics in frames of the reference system approach

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The new variant of the collective variables method for description the strong nonideal electron liquid model was suggested. Similarly to the Bohm-Pines method the Coulomb potential is splitted using θ-analogical functions on two parts: the long range and short range components $V_l(\mathbf{q}) = V_\mathbf{q} y(q|q_0)$; $V_s(\mathbf{q}) = V_\mathbf{q}\{1 - y(q|q_0)\}$, $V_\mathbf{q} = \frac{4\pi e^2}{q^2}$; $y(q|q_0) = 1 - \frac{2}{\pi}\mathrm{arctg}\left(\frac{q}{q_0}\right)^n$, where $n \geq 3$ and q_0 is a variative parameter.

We obtained the statistical operator representation in the extended space of individual variables (secondary quantization operators $a^+_{\mathbf{k},s}, a_{\mathbf{k},s}$) and collective coordinates using the transition operator. As the result of transition from collective variables to generation and annihilation operators of plasmons $b^+_\mathbf{q}$, $b_\mathbf{q}$ we get the electron-plasmon model of the electron liquid with the partition function $Z = \mathrm{Sp}_a\mathrm{Sp}_b\Big\{\hat{J}_{a,b}\exp[-\beta(\hat{H}_s + \hat{H}_p + \hat{H}_{ep})]\Big\}$. Where $\hat{H}_s$ is the hamiltonian of electrons with short-range interaction, $\hat{H}_p$ – the hamiltonian of interacting plasmons, $\hat{H}_{ep}$ – the operator of electron-plasmon interactions and operator $\hat{J}_{a,b}$ describe electron-plasmon relations.

To contrast to the standard perturbation theory in this approach the free electrons and noninteracting plasmons model is using as base system. Therefore in our approach the divaricate diagrams are absent and series decompositions have good convergence. The short-range interactions contribution was considered in the local-field approximation (calculations for the local-field function of electrons with short-range interactions are required).

The electron liquid model characteristics (correlation energy, binary distribution function, structure factor, local-field correction function) are calculated in $T = 0K$ case for wide range of the coupling parameter $(1 \leq r_s \leq 40)$.

The electron localized states in the screened charge field

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An certain interest to this problem is caused by a great value of applications in statistical physics of ionized systems, nuclear physics, scattering theory, astrophysics. We suggested two different variants for analytical solving of Schrodinger equation for the electron in a dot charge field with potential

$$V(r) = -z\frac{e^2}{r}\exp(-\varkappa\, r).$$

In the first case the equation for the radial function by the standard substitution $R(\rho) = \rho^l \omega_l(\rho)\exp(-\sqrt{-\varepsilon_l}\rho)$ is led to onedimensional integral equation for the function $\omega_l(\rho)$. For the case of radial function, which correspond to $1s$, $2p$, $3d$, $4f$,... electron states, the solution of this equation can be presented in the form of parametric integral of infinity dimension.

The condition $\omega_{l,0}(0|\sqrt{-\varepsilon_l}) = 1$ leads to the energy spectrum equation for the fixed orbital quantum number, which depends on dimensionless screening parameter $\xi = \varkappa\, a_0$. Another condition $\omega_{l,0}(0|0) = 1$ determines the critical values of parameter $\xi_{l,0}$, when the energy level passes in to continuous spectrum. The selfconsistens procedure of approximate factorization for integrals with infinity dimension is developed. On this base the energy levels and wave function dependence on ξ is investigated. A set of $\xi_{l,0}$ for the mentioned quantum states is calculated.

In the second case, which is applicable for any electron quantum states, the solution the differential equation for $\omega_l(\rho|\sqrt{-\varepsilon_l})$ is presented in the form of series $\omega_l(\rho|\sqrt{-\varepsilon_l}) = \sum\limits_{n=0}^{\infty} a_n^l(\xi|\sqrt{-\varepsilon_l})\rho^n$, where coefficients $a_n^l(\xi|\sqrt{-\varepsilon_l})$ are defined by the recurrent relations. By the exact and approximate summation of the asymptotic series the energy spectrum, wave function and critical values of the screening parameter $\xi_{l,n}$ for quantum states with any quantum numbers l, n are calculated.

Quasi-lattice approximation of statistical systems with strong superstable interactions

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A continuous infinite system of point particles interacting via two-body strong superstable potential is considered in the framework of classical statistical mechanics.

In the present report we propose some approximation of the main quantities, which describe macroscopical and microscopical characteristics of systems, such as grand partition function and correlation functions. The main idea is in the following: we split the space $\mathbb{R}^d$ into nonintersecting hyper cubes with a volume a^d and define approximated grand partition function and the family of approximated correlation functions in such a way, that they take into account only such configurations of particles in $\mathbb{R}^d$, when there is not more than one particle in each cube.

It was shown, that for the potentials which have non integrable singularity in the neighborhood of the origin(strong superstable potentials) the pressure of the approximated system converge to the pressure of the initial system if $a \to 0$ for any values of an inverse temperature $\beta > 0$ and a chemical activity z. The same result is true for the family of correlation functions in the region of small z.

This report is based on the article [1].

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Feshbach resonances and multiband superconductivity near the misfit strain quantum critical point in the 3D phase diagram oh high T_c superconductors

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The experiments on cuprates and FeAs superconductors have shown that the Global Phase Diagram requires a 3D phase diagram where the critical temperature T_c is dependent on two variables: the doping and the misfit strain called the Aeppli-Bianconi phase diagram. The material dependent variable is the internal chemical pressure due to the superlattice misfit strain between active layers and spacer layers that is an intrinsic physical parameter of superlattices at atomic limit. The mesoscopic phase separation regime has been called the SUPERSTRIPES regime where bubbles of incommensurate lattice, charge and spin ordering coexists with the superconducting phase. The maximum T_c of the HTcS is at the phase boundary of the mesoscopic phase separation. The commensurate normal stripes phase occurs in a region in the 2D space of charge density and misfit strain. The physics of high T_c superconductivity in FeAs multilayers shows a similar 3D phase diagram where the magnetic orthorhombic phase plays the role of commensurate stripes phase and disappears as a function of doping and pressure. The maximum T_c occurs at the phase boundary of the mesoscopic phase separation.

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