Annual Conference in Ukraine

Statistical Physics 2005:

Modern Problems and New Applications

28–30 August 2005, Lviv, Ukraine

BOOK OF ABSTRACTS

Lviv – 2005

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Institute for Condensed Matter Physics
of the National Academy of Sciences of Ukraine
Lviv, Ukraine

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National University
Lviv, Ukraine

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The aim of StatPhys2005 Conference is to renew the traditional annual Conferences on Statistical Physics established in Ukraine in the early 70ies of the last century. Remarkably, the Conference will take place in 2005 declared as the World Year of Physics by UNESCO. The timing of this conference is chosen to coinside with the 80th birthday of Prof. Ihor Yukhnovskii, one of the main organizers of a number of previous meetings in Statistical Physics and also the founder of the Lviv scientific school in condensed matter theory and statistical physics. The subject of the conference covers his main scientific interests.

The conference is addressed to physicists (experimentalists and theoreticians) working in the field of Statistical Mechanics and Condensed Matter Physics. Although our primary goal is to bring together Ukrainian scientists, the researchers from abroad working in the field of statistical physics are highly welcome to what, we believe, will promote an international collaboration.

Main topics

- Physics of liquids and soft matter theory
- Quantum many-particle systems
- Phase transitions and critical phenomena
- Exotic statistical physics

Contacts

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Statistical Physics 2005:

Modern Problems and New Applications

Programme

28–30 August 2005, Lviv, Ukraine

Sunday, August 28, 2005

9:15 – 9:30 Conference opening

PLENARY TALKS

Chaired by V.G. Baryakhtar

9:30 – 10:00 J.P. Badiali
The concept of entropy: From black hole to pre-relativistic systems

10:00 – 10:30 N.M. Plakida
Theory of superconductivity in cuprates

10:30 – 11:00 L. Pastur
Random matrix model of quantum relaxation

11:00 – 11:30 Coffee Break

PLENARY TALKS

Chaired by J.P. Badiali

11:30 – 12:00 H. Krienke
Dielectric and structural properties of solvent mixtures

12:00 – 12:30 D.Ya. Petrina
Stochastic and dissipative dynamics and Boltzmann equation

12:30 – 13:00 Yu.A. Izyumov
Generating functional approach in the theory of strongly correlated systems

13:00 – 13:30 O.S. Bakai
Thermodynamics and structure of mesoscopically heterophase systems. Many-species model

13:30 – 15:00 Lunch

15:00 – 17:00 SECTION SESSIONS

17:00 – 17:30 Coffee Break

17:30 – 19:00 SECTION SESSIONS

PLENARY TALKS

Chaired by A.G. Zagorodny

19:10 – 19:40 I. Mryglod
Yukhnovskii's contribution to the development of new methods of statistical physics

19:40 – 20:00 Presentation of the Book of Selected Yukhnovskii's Papers

20:20 – 22:00 GET-TOGETHER PARTY

SECTION SESSIONS 15:00 – 17:00

SECTION 1: **Physics of liquids and soft matter theory**
Chaired by M.F. Holovko

15:00 – 15:20 T.G. Mason
Extreme emulsification: formation and structure of nanoemulsions

15:20 – 15:40 B. Lev
Statistical physics of model system with interaction

15:40 – 16:00 T. Bryk*, I. Mryglod
Collective excitations in a binary metallic glass $Mg_{70}Zn_{30}$: A theoretical GCM study

16:00 – 16:15 F. Jiménez-Ángeles*, M. Lozada-Cassou, G. Odriozola
Electrolyte distribution around two like charged rods and their effective attractive interaction

16:15 – 16:30 O. Kalugin*, Ya. Kolesnik, A. Golubnychiy
Ion association in non-aqueous electrolyte solutions from a molecular modelling point of view

16:30 – 16:45 T. Patsahan*, M. Holovko
The liquid-vapour coexistence of simple fluids confined in disordered matrix: A new approach in the theory of associative fluids

16:45 – 17:00 A. Baumketner*, J.-E. Shea
Free energy landscapes for dimerization of amyloidogenic tetrapeptides

17:00 – 17:30 Coffee Break

SECTION SESSIONS 15:00 – 17:00

SECTION 2: **Quantum many-particle systems**
Chaired by I.V. Stasyuk

15:00 – 15:20 V. Adamyan
Correlation functions of 2D and 1D electron gas

15:20 – 15:40 N.N. Bogolubov, Jr.*, A. Soldatov, S. Kruchinin
Method of intermediate problems in the theory of two-dimensional quantum dots formed by Gaussian confining potentials in the presence of a magnetic field

15:40 – 16:00 A. Honecker
Magnetocaloric effect in frustrated spin systems

16:00 – 16:15 H. Gomonay*, V. Loktev
Magnetoelastic mechanism of the domain formation in antiferromagnets

16:15 – 16:30 R. Hasan, M. Kartsovnik, V. Peschansky*
Hall effect in organic layered conductors

16:30 – 16:45 Yu. Fridman, O. Kosmachev, Ph. Klevets, O. Kozhemyako
Phase transitions in 2D XY-model with biquadratic exchange interaction

16:45 – 17:00 P. Kostrobij, B. Markovych*, Yu. Suchorski
Calculation of electron-density profiles of semibounded metal, which is placed in external electric field

17:00 – 17:30 Coffee Break

SECTION SESSIONS 15:00 – 17:00

SECTION 3: **Phase transitions and critical phenomena**
Chaired by R. Folk

15:00 – 15:20 A. Kozak, Yu. Kozitsky*
Non-Gaussian fixed points in the method of I.R. Yukhnovskii

15:20 – 15:40 M. Jaščur, J. Strečka*
Reentrant transitions of a mixed spin-1/2 and spin-1 Ising model on the diced lattice

15:40 – 16:00 I. Omelyan*, W. Fenz, I. Mryglod, R. Folk
XY-spin fluids in an external magnetic field: an integral equation approach

16:00 – 16:15 Yu.G. Medvedevskyh
Conformation of intertwining polymeric chains in the concentrated solutions and melts in the self-avoiding random walks statistics

16:15 – 16:30 M. Korynevskii*, V. Solovyan
Ferroelectric-antiferroelectric mixed systems. Equation of state, thermodynamic functions

16:30 – 16:45 D. Ivanejko, J. Ilnytskyi, B. Berche, Yu. Holovatch
Simulational studies of the random-site Ising model criticality

16:45 – 17:00 A.N. Vasil'ev, A.V. Chalyi
Critical parameters and pair correlations in confined multicomponent liquids

17:00 – 17:30 Coffee Break

SECTION SESSIONS 17:30 – 19:00

SECTION 2: **Quantum many-particle systems**
Chaired by F. Mancini

17:30 – 17:50 I.M. Dubrovskii
Diamagnetism of electron gas

17:50 – 18:10 O. Derzhko*, V. Myhal
A microscopic theory of photonucleation: Density functional approach for the properties of a fluid of two-level atoms, a part of which is excited

18:10 – 18:30 D. Fil, S. Shevchenko
Superflow of electron-hole pairs in quantum Hall bilayers: the role of interlayer tunneling

18:30 – 18:45 A. Brandt, A. Grigoriev, V. Ilyin
Multilevel simulations of macromolecules

18:45 – 19:00 Yu. Skorenkyy*, O. Kramar, Yu. Dovhopyaty
Energy spectrum of the organic quasi-1D conductor with NNN and correlated hopping

SECTION SESSIONS 17:30 – 19:00

SECTION 3: **Phase transitions and critical phenomena**
Chaired by J.M. Caillol

17:30 – 17:50 A.D. Alexeev*, E. Ulyanova, N. Kalugina, S. Degtyar
Phase transitions in the coal-water-methane system

17:50 – 18:10 O. Patsahan*, I.M. Mryglod, J.-M. Caillol
Charge-charge correlations near gas-liquid critical point

18:10 – 18:30 R.M. Yevych, Yu.M. Vysochanskii*
Lattice dynamics and phase transitions in $Sn_2P_2S(Se)_6$ ferroelectrics

18:30 – 18:45 J. Strečka
Non-universal critical behavior of a mixed-spin Ising model on the generalized Kagomé lattice

18:45 – 19:00 W. Fenz*, R. Folk, I. Omelyan, I. Mryglod
Phase behavior of Ising mixtures

SECTION SESSIONS 17:30 – 19:00

SECTION 4: **Methods and exotic problems of statistical physics**
Chaired by O.S. Bakai

17:30 – 17:50 A. Olemskoi*, S. Kokhan
Effective temperature of self-similar time series

17:50 – 18:10 Yu.G. Rudoy, A.D. Sukhanov
The geometric representations in classical and statistical equilibrium thermodynamics (contact, Riemann and information geometrics)

18:10 – 18:25 A. Khomenko
Synergetics of phase dynamics of ultrathin lubricant film

18:25 – 18:40 V. Ignatyuk*, M. Tokarchuk, P. Kostrobij
Kinetic equations approach to the description of chemical reactions between adparticles at a metallic surface

18:40 – 18:55 R. Bobrov*, V. Kulinskii
Collective behavior of self-propelling particles in a circle with reflecting boundary conditions

Monday, August 29, 2005

PLENARY TALKS

Chaired by I.R. Yukhnovskii

9:00 – 9:30 J.-M. Caillol*, O. Patsahan, I. Mryglod
The collective variables representation of simple fluids from the point of view of statistical field theory

9:30 – 10:00 V.M. Kalita, V.M. Loktev
Quantum (meta)magnetic transitions in Ising model with single-ion anisotropy

10:00 – 10:30 N.F. Shulga
Dynamical chaos phenomenon at passing of fast charged particles through oriented crystals

10:30 – 11:00 M. Holovko
Statistical theory of electrolyte solutions

11:00 – 11:30 Coffee Break

11:30 – 13:30 SECTION SESSIONS

13:30 – 15:00 Lunch

PLENARY TALKS

Chaired by Yu.A. Izyumov

15:00 – 15:30 I.V. Baryakhtar, V.G. Baryakhtar*
Limitations for applications of the detail balance principle

15:30 – 16:00 F. Mancini
Fermionic systems with charge correlations

16:00 – 16:30 I.O. Vakarchuk
A self-consistent theory of liquid ^{4}He. Variational approach

16:30 – 17:00 M. Dudka, R. Folk*, Yu. Holovatch, G. Moser
Critical dynamics of generalized model C

17:00 – 17:30 Coffee Break

17:30 – 19:00 POSTER SESSION

Chaired by B. Berche,
N.N. Bogolubov, Jr.,
E.G. Petrov,
N.F. Shulga

20:00 – 22:00 CONFERENCE DINNER

SECTION SESSIONS 11:30 – 13:30

SECTION 1: **Physics of liquids and soft matter theory**
Chaired by H. Krienke

11:30 – 11:50 V. Lisy*, J. Tothova, A. Zatovsky
The joint Rouse-Zimm theory of the dynamics of polymers in solutions

11:50 – 12:10 A. Trokhymchuk
Structural interactions and "softness" of the matter

12:10 – 12:30 V. Vikhrenko*, G. Bokun, D. Gapanjuk, Y. Groda, R. Lasovsky
Equilibrium and diffusion properties of lattice gas systems

12:30 – 12:50 J. Kupriyanova*, A. Zatovsky
Light scattering studies on the particles with permanent and induced dipole moments in solutions

12:50 – 13:05 L. Bulavin, N. Malomuzh, K. Pankratov*
Thermal motion in normal and supercooled water according to data of quasi-elastic incoherent neutron scattering

13:05 – 13:20 M. Druchok*, M. Holovko, T. Bryk
Primitive model for cation hydrolysis: A molecular dynamics study

13:20 – 13:35 V.V. Ryazanov*, S.G. Shpyrko
First-passage time: a conception leading to superstatistics

13:30 – 15:00 Lunch

SECTION SESSIONS 11:30 – 13:30

SECTION 2: **Quantum many-particle systems**
Chaired by N.M. Plakida

11:30 – 11:50 V. Shvets*, S.Savenko
Conductivity of metallic hydrogen

11:50 – 12:10 A.M. Shvaika*, O. Vorobyov, J.K. Freericks, T.P. Devereaux, M. Jarrell
Dynamical cluster studies of nonresonant Raman scattering in the Falikov-Kimball model

12:10 – 12:30 S. Peletminskii, A. Peletminskii, Yu. Slyusarenko, A. Sokolovsky
Generalized Gross-Pitaevskii equations for $T \neq 0$ with taking into account binary correlations of the Bose condensate particles

12:30 – 12:45 V. Kopylets, S. Kornii, V. Pokhmurskii
Electronic structure of large modified nickel nanoclusters

12:45 – 13:00 R. Levitskii, S. Sorokov*, A. Vdovych, Z. Trybula, V. Schmidt
Thermodynamics and relaxational properties of the $Rb_{1-x}(NH_4)_xH_2PO_4$-type proton glasses

13:00 – 13:15 Yu.K. Rudavskii, G.V. Ponedilok, M.I. Klapchuk
Influence of the structural disorder on impurity states in liquid metal

13:15 – 13:30 V. Khodusov*, D. Litvinenko
Thermoelectromechanical waves in superfluid Helium

13:30 – 15:00 Lunch

SECTION SESSIONS 11:30 – 13:30

SECTION 4: **Methods and exotic problems of statistical physics**

Chaired by C. von Ferber

11:30 – 11:50 V. Demutskiy, O. Pignastiy
Synergetic economics of the manufacturing firm with mass production output

11:50 – 12:10 C. von Ferber, Yu. Holovatch*, V. Palchykov
Are public transport networks scale-free?

12:10 – 12:30 V.I. Gerasimenko
On the rigorous derivation of kinetic equations

12:30 – 12:45 D. Kharchenko*, A. Olemskoi, I. Knyaz'
Nonequilibrium phase transitions in stochastic systems induced by noise cross-correlations

12:45 – 13:00 Yu. Slyusarenko, A. Sokolovsky, S. Sokolovsky
Kinetics of a system in external random field with small correlation time. Higher order approximation

13:00 – 13:15 A. Chechkin*, V. Gonchar
Origin and applications of fractional kinetic equations

13:15 – 13:30 A. Antoniouk, A. Antoniouk
Nonlinear effects in the regularity problems for infinite dimensional evolutions of classical Gibbs models

13:30 – 15:00 Lunch

Tuesday, August 30, 2005

PLENARY TALKS

Chaired by V.M. Loktev

9:00 – 9:30 B. Berche
Nematic phase transitions in two-dimensional systems

9:30 – 10:00 A.M. Kosevich
Excitation spectrum and electrical properties of the condensate of Bose-atoms

10:00 – 10:30 I.V. Stasyuk
Phase transitions and instabilities in strongly correlated systems with local lattice anharmonicity

10:30 – 11:00 E.G. Petrov
The kinetics of current formation through a single molecule

11:00 – 11:30 Coffee Break

PLENARY TALKS

Chaired by A.M. Kosevich

11:30 – 12:00 N.N. Bogolubov, Jr.
Approximation in polaron theory for Fröhlich-type system

12:00 – 12:30 A. Zagorodny*, V. Zasenko, J. Weiland
Diffusion and stochastic particle acceleration in strong random fields

12:30 – 13:00 C. von Ferber
Statistical physics of complex networks

13:00 – 13:30 M.P. Kozlovskii
Development and application of the Yukhnovskii's phase transition theory for description of 3D-statistical systems

13:30 – 15:00 Lunch

PLENARY TALKS

Chaired by L. Pastur

15:00 – 15:30 M. Lozada-Cassou*, G.E. Aguilar, F. Jiménez-Ángeles, G. Odriozola
Statistical mechanics of confined charged fluids

15:30 – 16:00 S. Peletminskii, Yu. Slyusarenko*
Second quantization method in the presence of bound states of particles

16:00 – 16:30 M.S. Gonchar
Information model of economy

16:30 – 17:00 I.R. Yukhnovskii
Thermodynamic analogies in economics

17:00 – 17:30 CLOSING OF THE CONFERENCE

Statistical Physics 2005:

Modern Problems and New Applications

Plenary Lectures

28–30 August 2005, Lviv, Ukraine

The concept of entropy: From black hole to pre-relativistic systems

J.P. Badiali

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The concept of entropy is one of the most important in thermodynamics. After Boltzmann, entropy became the key quantity on which statistical mechanics can be found. Today, as a result of the black hole theory, there is a large and deep discussion about the real meaning of entropy. In a lot of papers the authors try to associate the black hole entropy with the counting of a number of microstates in the spirit of Boltzmann. However after thirty years of intensive works in this domain we are still to deal with very basic questions such as which kind of microstates are involved in this entropy and where these states are located. In this talk we consider some results of black hole thermodynamics as firmly established and at least some of them can be reformulated in a very general manner. Consequently it seems natural to ask if some of these results might be extended to ordinary systems for which a pre-relativistic description is sufficien [1].

Here we focus on two black hole results. First, we show that it exists a general relation between time and temperature and its derivation is even more general that the one used in black hole physics. Second, we show that it exists a general relation between action and entropy. These results have been established starting from a spacetime description of ordinary physics [2]. This work suggests that it should exist a general definition of entropy directly connected with the spacetime structure, of course for ordinary system this definition gives the same result than the one based on the use of the Boltzmann definition.

1. Badiali J.P. arXiv gr-qc /0505050
2. Badiali J.P. J. Phys. A Math. Gen., 2005, **38**, 1; arXiv quant-ph/0409138

Thermodynamics and structure of mesoscopically heterophase systems. Many-species model

O.S. Bakai

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Heterophase fluctuation model taking into account frustrations of the fluctuons is used for considerations of the mesoscopically heterophase systems. Equilibrium equations for fluctuons of a mesoscopic scale are deduced. Impact of the frustrations on the phase equilibrium and on the mode of liquid solidification is investigated. It is pointed out that the frustrations have an essential influence on formation of the long-range correlated fractal heterogeneities (the Fischer cluster) in liquids and on polyamorphous transformations of glasses. Definition of isostructural and non-isostructural polyamorphism is introduced and the kinetic constrain of the polyamorphous transformation is formulated.

To consider the criticality and critical fluctuations of the mesoscopically heterophase systems in continuum mean field approximation, the random field free energy functional of the Ginzburg-Landau type is deduced. It is shown that the systems of this type possess a new criticality properties and that in the critical point (end point on the coexistence curve) a first order phase transition takes place.

As an example three-species model is considered in detail. Discussion of experimental data and theoretical models devoted to the problem considered are included.

Limitations for applications of the detail balance principle

I.V. Baryakhtar, V.G. Baryakhtar

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The problem of collision integral construction was studied for two cases: solitons and usual particles. The case of solitons is a case when the exact solution of scattering problem is known. It gives us a principal possibility to find the expression for soliton — solitons collision integral. This expression for the collision integral is a one that does not satisfy the detail balance principle. This unusual situation is connected with the fact that exact expression for the collision integral consists of two part: that which presents the renormalization of solitons velocity due to their interaction, and the part which is responsible for the entropy production. We present here the method of separation both these parts from initial formula for the collision integral.

We revised the problem of construction of the collision integral and the detail balance principle in the case of usual particles. It is shown that the detail balance principle takes place only in the case when the sizes of particles are equal to zero. For the case of finite size particles the detail balance principle is satisfied only in the frame of corrections $r_0 \ll l$, where r_0 is the radius of atoms and l is the scale of non-homogeneity of the distribution function.

Nematic phase transitions in two-dimensional systems

B. Berche[a,b]

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Simulations of nematic-isotropic transition of liquid crystals in two dimensions are performed using $O(n)$ vector models. The models consist in a generalisation of XY and Heisenberg models. They are characterised by non linear nearest neighbour spin interaction governed by the fourth Legendre polynomial P_4 but have two different spin symmetries ($O(2)$ and $O(3)$). The systems are studied through standard Finite-Size Scaling and conformal rescaling of density profiles or correlation functions. The nature of the transition is shown to be strongly dependent of the spin symmetry. The low temperature limit is discussed in the spin wave approximation and confirms the numerical results.

Approximation in polaron theory for Fröhlich-type system

N.N. Bogolubov, Jr.

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The functional variational method, which is based on the T-product formulation, is developed. This method uses the linear polaron model as a trial one and allows to obtain an upper bound limit for the free energy (and the energy of ground state as well) in the case of the Fröhlich-type model system, which is valid for all the values of the model parameters and temperature. An approach, based on the T-product averages, could be considered as realization of Feymann's idea of path integrals on more rigorous level. We also studied a weak interaction limit with systematic finite-temperature perturbation, based on the same T-product averages formulation as well as on adiabatic perturbation approach, which is valid for the strong coupling case.

The collective variables representation of simple fluids from the point of view of statistical field theory

J.-M. Caillol[a], O. Patsahan[b] and I. Mryglod[b]

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[b] *Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine 1 Svientsitskii Str., 79011 Lviv Ukraine*

The collective variable representation (CV) of classical statistical systems such as simple liquids has been intensively developed by the Ukrainian school after seminal works by Prof. Ihor Yukhnovskii. The basis and the structure of the CV representation are reexamined here from the point of view of statistical field theory and compared with another exact statistical field representation of liquids based upon a Hubbard-Stratonovich transform. We derive a two-loop expansion for the grand potential and free energy of a simple fluid in both version of the theory. The results obtained by the two approaches are shown to coincide at each order of the loop expansion. The one-loop results are identical to those obtained in the framework of the random phase approximation of the theory of liquids. However, at the second-loop level, new expressions for the pressure and the free energy are obtained, yielding a new type of approximation. Recent applications of the formalism to an understanding of the critical behavior of ionic fluids is also briefly discussed.

Critical dynamics of generalized model C

M. Dudka[a,b], R. Folk[b], Yu. Holovatch[c,a,b], and G. Moser[d]

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[c] *Ivan Franko National University of Lviv, Ukraine, E–mail: hol@ph.icmp.lviv.ua*

[d] *Institute for Physics and Biophysics, University of Salzburg, Austria*

In model C a real relaxing order parameter (OP) is statically coupled to a conserved (diffusing) density. The critical behavior of this model has been resolved only recently [1]. We consider two generalizations of model C: (i) we couple two conserved densities to the relaxing complex order parameter (model C$^{*\prime}$) instead of one, and (ii) we introduce disorder within model C.

In case (i) a transformation to 'orthogonalized' densities can be performed where only one secondary density with nontrivial static coupling to the OP exists while the second one remains Gaussian. The secondary densities remain dynamically coupled by the nondiagonal diffusion coefficent. General relations for the field theoretic functions allow to relate the *asymptotic* critical properties of model C$^{*\prime}$ to the simpler model C. The *nonasymptotic* properties however differ as can be seen from the flow of the dynamic parameters, which is presented for the case of a real OP with componets $n = 1, 2, 3$ [2].

In case (ii) it is known, that the secondary density has no effects on the asymptotic critical behavior of order parameter of disordered system, therefore its *asymptotic* dynamical properties reduce to those of model A. However, disorder affects considerably the *nonasymptotic* dynamical behavior. We present the effective critical behavior in two loop order [3], which is relevant in the comparison with experiment or Monte Carlo simulations.

Supported by the Austrian Fonds zur Förderung der wissenschaftlichen Forschung, project No 15247-PHY and No 16574-PHY.

1. R. Folk, G. Moser Phys. Rev E **69**, 036101 (2004)
2. R. Folk, G. Moser Phys. Rev E **71**, February (2005).
3. M.Dudka, R. Folk, Yu. Holovatch, G. Moser, preprint (2005)

Statistical physics of complex networks

C. von Ferber

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The theory of networks (in mathematical terms: graphs) has had an explosive development recently, triggered by the discovery that the structure of many networks like the world-wide-web, biological systems such as the cell metabolism and food webs, as well as communication , traffic and social networks diplay similar scaling behavior. The key to this development is the description of these systems as evolving networks that display a much larger number N(k) of vertices with high number k of links than one would expect from a model of random networks, where this number N(k) decays faster that exponentially with k. In contrast, for many real world networks N(k) exhibits a power law, namely $N(k) \sim k^{-\gamma}$ holds. Networks for which this relation is fulfilled are called *scale-free*. This property indicates critical behavior and indeed these networks can be understood as non-equilibrium growing systems that self-organize into scale free structures [1] displaying self-organized criticality. The properties of scale-free networks, in particular percolation, differ markedly from the classical case: for slowly decaying distributions ($\gamma < 4$) nontrivial γ-dependent critical exponents appear.

More recently, also the dynamics of such networks is explored. Many problems ranging from the dynamics of randomly branched polymers [2] and the stress relaxation of near critical gels, over random resistor-capacitor networks to glassy relaxation dynamics, depend on the discrete Laplacian $\mathbf{A}$ defined on the network. Specializing to scalefree networks with degree distributions $p_k \sim k^{-\gamma}$ the dynamical spectrum is accessible by analytic methods [3] and one finds characteristic changes in the dynamical spectrum $\rho(\lambda)$ when lowering γ to $\gamma < 4$ i.e. from fast to slower decaying degree distributions.

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Information model of economy

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Economic reality puts the problems that can be solved only within new paradigm. In the report, we shall expose new mathematical results on the construction of the new mathematical model describing economic systems. We present:
i) axioms of choice by costumers and decision by firms accounting for stochasticity of costumer's choices and their interdependence, stochasticity of firms decisions and their interdependence;
ii) introduced new mathematical objects describing costumer's choices and firms decisions — costumer choice and firm decision random fields;
iii) introduced new concept of complete description of costumer choice accounting for the information about available states of the economic system and evaluation of this information by costumers during the choice;
iv) formulation of costumer choice and firm decision axioms and construction of unique probability space on which the existence of costumer choice and firm decision random fields is proven;
v) the constructive theory of costumer choice random fields on the base of introduced new concepts, namely conditionally independent random fields by which the new concept of the random field of consumer information evaluation is introduced determining the structure of costumer choice; random field of consumer information evaluation is the evaluation of available information about the state of economic system influencing the choice;
vi) established general expression for the random fields of consumer choice in terms of random fields of information evaluation by the consumer and random fields of firms decision;
vii) established geometrical structure of convex down and continuous from up after Kakutani technological mappings and the theorem on the existence of continuous firm behavior strategy arbitrarily near in profit to optimal behavior strategy;
viii) constructed theory of economic equilibrium for proposed economic models in uncertainty conditions;
ix) constructed algorithms to find equilibrium states in proposed models of the economy in uncertainty conditions.

Statistical theory of electrolyte solutions

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For the last fifty years the electrolyte solutions were the polygon for the development and the application of new approaches in the theory of liquids state and soft matter. In this report some aspects of the electrolyte solution theory will be reviewed. Special attention will be focused on the analysis of the activity of I.R. Yukhnovskii and his coworkers on the studies of the screening effects in the systems with electrostatic interactions, the development of the plasma-parameter and the cluster expansions for pair distribution functions of ionic systems, the idea of the treatment of short-range interionic interactions as the reference system in the theory of ionic fluids and the development of the ion-molecular approach for the correct description of solvation phenomena in electrolyte solutions.

Finally a few modern aspects in the statistical theory of electrolyte solutions will be illustrated. Between them the development of the ionic association concept for the treatment of a different types of clusterization in electrolyte solution. The capabilities of this approach will be illustrated by the description of thermodynamic, dielectric and transport properties of electrolyte solutions in weakly polar solvents, the explanation of the anomalous temperature dependence of the capacitance of the electrical double layer and the treatment of the effect of electrolyte on the rate of intramolecular electron transfer.

Our last results of the modeling of the effects of cation hydrolysis and polynuclear ion formation in aqueous solutions of heavy metal salts, molecular treatment of mesoscopic correlations in aqueous surfactant solutions, the specific of the screening effects in ionic and ion-molecular fluids adsorbed in a disordered charged and dielectric matrices will be also considered.

Generating functional approach in the theory of strongly correlated systems

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Basic models in the theory of magnetism and strongly correlated electron systems (models of Heisenberg, Hubbard, Anderson, sd–model) are studied by method of the generating functional which is a generalization of Kadanoff-Baym approach on Hamiltonians expressed in the terms of spin and X-operators. Difficulties are connected with the fact that these operators do not commute on c-value unlike to the conventional Fermi-operators.

For each of the model we derived equation for one-particle Green's function in terms of the functional derivatives over fluctuating fields depending on space and thermodynamical time. The structure of equations for the different models is turned out to be similar. It reflects the similarity of permutation relations for spin- and X-operators. A multiplicative representation for Green's functions introduces the terminal and self-energy parts, and equations with the functional derivatives for them are derived for each of the model. Iterations of this equations produce a perturbation theory nearly atomic limit.

Analysis of first two steps of the iterations for the terminal and self-energy parts allows to introduce a mean field approximation for the model and leads to a metal-insulator phase transition in the Hubbard model and the Periodic Anderson model. Green's functions in the bosonic sector describe collective modes in the models.

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Quantum (meta)magnetic transitions in Ising model with single-ion anisotropy

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The Ising model with single-ion anisotropy of "easy-plane" type in external longitudinal magnetic field is considered. It is shown that the transition from an initial antiferromagnetic state of a system to the final ferromagnetic (paramagnetic) one is occurred through the sequence of metamagnetic quantum transitions. The evidently observable jumps of the sampme magnetization take place at rather low temperatures, and their number depends on paramagnetic ion spin value S. The difference between critical magnetic fields values is defines by the single-ion anisotropy and intra-sublattice exchange parameters and do not depend upon intersublattice one. The attempt is made to compare the results obtained with the experimentally observed (meta)magnetic transition in low dimensional Ising systems – nikelites.

Excitation spectrum and electrical properties of the condensate of Bose-atoms

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It is shown that the condensate of a degenerated Bose-gas consisting of neutral atoms possesses electrical properties which differ from a trivial polarisation of the atoms in an electric field. A notion of an isotropic quadrupole moment (IQM) of a neutral atom is introduced [1]. The isotropic quadrupole moment of the atoms produces a distribution of the electric potential which reflects a specific space ordering in the condensate. The additional term in the Gross-Pitaevskii equation is found which is responsible for the account of the electrical activity of neutral atoms, and a new type of the nonlinear Schroedinger equation (NSE) is constructed. Small vibrations of the Bose-gas are considered and a correction to the Bogolubov spectrum of elementary excitations in the degenerated Bose-gas is obtained. A new term in the Bogolubov formula for the spectrum is proportional to the condensate density and $(ak)^4$ where a is the atom radius and k is the wave-vetor of an elementary excitatuion. Since the Bose-condensate is akin to the superfluid component in He II, a manifistation of its electrical activity could have a relation to the electrical activity of the superfluid liquid observed experimentally [2].

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Development and application of the Yukhnovskii's phase transition theory for description of 3D-statistical systems

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The main features of the suggested by I.R. Yukhnovskii [1] microscopic approach for describing phenomena in 3D systems near the critical point are presented. This approach is the realization of the universality hypothesis of Kadanoff [2] on the microscopic level. It is based on the use of the non-Gaussian distributions of order parameter fluctuations. This feature distinguishes this method from the well-known K. Wilson approach [3]. The attention is focused on the magnets with one- and multi-component order parameter, the general hierarchical model of magnet, ferroelectrics, the gas-liquid critical point, the phase separation transitions and others. The method allows one to obtain the explicit expressions [4] for the order parameter, susceptibility, heat capacity and other characteristics near the phase transition point.

The generalization of description of critical behaviour at the presence of the external field is the object of given research. The main physical characteristics of the one- component magnet in the vicinity of the phase transition point are analyzed for two cases of weak and strong magnetic fields. Near the critical point, the crossover from the temperature to field dependence is shown for such quantities as order parameter, susceptibility, and heat capacity.

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Dielectric and structural properties of solvent mixtures

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Mixtures of molecular solvents are investigated in the framework of Monte Carlo (MC) simulations and SSOZ integral equation techniques on the molecular Born-Oppenheimer (BO) level with classical interaction site models (ISM). Kirkwood-Buff integrals, Helmholtz energies and chemical potentials are discussed in the framework of different approaches as well as the calculation of dielectric constants of solvent mixtures.

Statistical mechanics of confined charged fluids

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Unsymmetrical electrolytes and macroions solutions confined by cavities of different geometries are studied. In particular the ionic structure inside and outside the cavity is calculated and analyzed. Other phenomena as the pressure, overcharging, charge separation, charge reversal are addressed.

Fermionic systems with charge correlations

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A system of localized particles, satisfying the Fermi statistics and subject to finite-range interactions, can be exactly solved in any dimension. In fact, in this case it is always possible to find a finite closed set of eigenoperators of the Hamiltonian. Then, the hierarchy of the equations of motion for the Green's functions eventually closes and exact expressions for them are obtained in terms of a finite number of parameters. For example, the method is applied to the study of the Ising model with spin 1/2, 1, 3/2, and to the Hubbard model with intersite Coulomb interaction in the ionic limit. For these models the relevant Green's functions and correlation functions are exactly calculated and depend on a finite set of parameters to be self-consistently determined. By means of algebraic constraints, such parameters are calculated in the one-dimensional case and the behavior of the relevant physical properties is reported.

Yukhnovskii's contribution to the development of new methods of statistical physics

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Since 50ies Ihor Yukhnovskii works in the field of statistical physics and condensed matter theory. His activity in this field [1] results in: development of several new methods in many-particle theory of classical and quantum systems; appearance of numerous important results in condensed matter physics; and creation of Lviv school of statistical physics, known now in many research centers all over the world.

In this report, the main emphases is made on the new methods proposed and developed by Prof. I.Yukhnovskii in 50-70ies years of the last century. Some of them are known and well described in the literature, but another ones were not published in English, so that general overview, performed in comparison with approaches of other authors, is required.

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Random matrix model of quantum relaxation

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We consider a two level system, $\mathcal{S}_2$, coupled to a general n level system, $\mathcal{S}_n$, via a Gaussian random matrix. We derive an integral representation for the mean reduced density matrix $\rho(t)$ of the small system $\mathcal{S}_2$ for different types of $\mathcal{S}_n$ in the limit $n \to \infty$. In particular, we identify models of $\mathcal{S}_n$ which can be considered as thermal reservoirs. In the limit $n \to \infty$ these yield, for suitable initial states of $\mathcal{S}_n$, a Gibbs form of $\rho(t)$ when $t \to \infty$. In the van Hove limit we obtain a master equation (Markov dynamics) for the evolution of $\rho(t)$ on appropriate time scales.

Second quantization method in the presence of bound states of particles

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The goal of this work was to develop a microscopic approach for describing the physical processes in many-particle systems in the presence of bound states of particles. To achieve this goal we developed a secondary quantization method for systems containing the bound states of particles.

The Fock space was introduced in the secondary quantization formalism. In this space the creation and annihilation operators of elementary particles and their bound states were introduced on an equal basis. The operators of the basic physical quantities acting in this space including the Hamiltonians of interactions of elementary particles and their bound states were constructed. It was shown that in the approximation of a "small radius of interaction" the above mentioned Hamiltonians transform into the well-known Hamiltonians for Coulomb's and dipole interactions between the particles of various kinds. The non-relativistic quantum electrodynamics of charged particles and neutral particles (the bound states) was constructed. Various physical effects including the theory of the van der Waals forces that act between atoms were considered as the approbation of the developed formalism. The description of such effects within the usual formalism requires more considerable efforts associated with introduction of interactions for neutral currents of bound states with electromagnetic fields.

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Stochastic and dissipative dynamics and Boltzmann equation

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The stochastic dynamics is obtained as the Boltzmann-Grad limit of the Hamiltonian dynamics of hard spheres. The stochastic Boltzmann hierarchy for sequence of correlation functions is derived. The one-particle correlation function is solutions of the Boltzmann equation. The stochastic Kac's dynamics in momentum space is derived from the stochastic dynamics in phase space.

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The kinetics of current formation through a single molecule

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Using the method of nonequilibrium density matrix for an open quantum system, the kinetics of electron transfer through a single molecule is studied with accounting for the Coulombic interaction between the transferred electrons. It is shown that a noted interaction becomes responsible for the appearance of different type of electron–transfer channels. Each channel is associated with fixed number of electrons captured by a molecule in the course of electron transmission. Electron transmission along the channel includes two different pathways. The first one reflects inelastic electron hopping between the electrodes and the molecules. At such a hopping just molecular states with different number of captured electrons participate in formation of the current as real intermediate states. The number of captured electrons is defined by electrode–molecule transfer rates which, in turn, depend on the number of captured electrons. Therefore, single–electron distribution functions are derived from solution of nonlinear kinetic equations. Second electronic pathway includes a direct electron transmission between the electrodes. In this case, the noted molecular states create an effective electrode–electrode coupling. This coupling provides a coherent mechanism of an electron transfer through a molecule. But, owing to a kinetic occupation of the molecule by the transferred electrons the transmission along elastic coherent pathway is controled by inelastic hopping process. The detail analyzis of electron transmission is carried out for a molecule with isolated energy levels. It allowed to derive analytic expressions for both elasic and inelastic components of the current. Based on these analytic results various transmission regimes are analyzed including the rectification regime.

Theory of superconductivity in cuprates

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A microscopic theory of superconductivity mediated by antiferromagnetic (AF) exchange and spin-fluctuations within the effective $p-d$ Hubbard model is developed. By applying the Mori-type projection technique for the (4×4) matrix Green function in terms of the Hubbard operators, the Dyson equation is derived [1]. In the mean-field approximation (MFA) the anomalous correlation functions $\langle c_{i\downarrow} c_{i\uparrow} N_j \rangle$ describe pairing on one lattice site but in the different Hubbard subbands. It is proved, by a direct calculation of these functions *without any decoupling*, that the pairing in MFA is mediated by the conventional AF exchange interaction J as in the t-J model. The retardation effects for this pairing which stems from the *interband hopping* with large charge transfer excitation energy, are negligible that results in the pairing of all charge carriers with high T_c proportional to the Fermi energy μ: $T_c^{(ex)} \simeq \sqrt{\mu(W-\mu)}\exp(-1/V_{ex})$ where W is the renormalized bandwidth and $V_{ex} = JN(\mu)$ is the coupling constant. The self-energy calculated in the noncrossing approximation describes the spin-fluctuation pairing in the energy shell $\pm\omega_s$ induced by the *intraband hopping*. By taking into account both pairing channels, we can write for the superconducting temperature an estimate

$$T_c \simeq \omega_s \exp(-1/\tilde{V}_s), \quad \text{where} \quad \tilde{V}_s = V_{sf} + V_{ex}/[1 - V_{ex}\ln(\mu/\omega_s)],$$

which gives $T_c \simeq 160$ K for $\mu = W/2 \simeq 0.35$ eV, $\omega_s \simeq J \simeq 0.13$ eV and weak coupling $V_{sf} \simeq V_{ex} = 0.2$. Numerical solution of the gap equation proves d-wave gap symmetry and determines T_c dependence on the hole concentration which agrees with experiments in cuprates. The theory explains small oxygen isotope effect and T_c dependence on the lattice constant (pressure) in mercury cuprates [2]. Comparison with the results for the t-J model [3] is given.

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Dynamical chaos phenomenon at passing of fast charged particles through oriented crystals

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Crystal has a regular structure, therefore it seems at first sight that any movement of particle in a crystal must be regular. In fact, this is not the case. Along with a regular one, the motion of a particle in a crystal can be chaotic relatively to the strings of atoms of a crystal. The report presents some results of theoretical studies of the dynamical chaos phenomenon at the motion of charged particles in a periodical field of atomic strings of a crystal, as well as the manifestation of dynamical chaos at process of coherent radiation by relativistic electrons in a crystal. A possibility of anomalous phenomena at diffusion of fast charged particles in the periodical field of atomic strings of a crystal is shown.

Phase transitions and instabilities in strongly correlated systems with local lattice anharmonicity

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In the lecture the problems of theoretical description of physical effects in systems with strong electron correlations, where the locally anharmonic structure elements are present and are characterized by the double-well potential, are discussed. We use models which are based on the pseudospin formalism and include the Hubbard-type electron interactions. Among them, the pseudospin-electron model (PEM), which can be considered as an extension of the Falicov-Kimball (FK) model due to inclusion of proper dynamics (of the tunneling type) of pseudospins is the main object of interest.

We give a review of results obtained at the study of thermodynamics and energy spectrum of such systems in the framework of PEM. Consideration is performed on the basis of generalized random phase approximation (GRPA) and dynamical mean field theory (DMFT). Cases of strong and weak pseudospin-electron coupling as well as infinitely large or absent Hubbard correlation are considered. The model is generalized also on the two-sublattice case. There are described: the phase transitions, connected with the jump-like changes of electron concentration and pseudospin mean value (that correspond to the change of occupancy of local positions); the transitions to phases with commensurate or incommensurate modulation; the instabilities with respect to separation into different (uniform or modulated) phases. A possibility of realization of superconducting phase and the metal-insulator transition in PEM is investigated. The corresponding phase diagrams are built. They are compared with the phase transition diagrams for the FK and anharmonic Holstein model. Peculiarities of the electron spectrum and the low-frequency pseudospin excitation spectra are analyzed.

The applications of the PEM (and its more complicated versions) to the study and description of nonuniform states, structure instabilities and modulated structures in high-T_c superconductors as well as energy spectra and phase transitions in other strongly correlated anharmonic systems are discussed.

A self-consistent theory of liquid ^{4}He. Variational approach

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A method of the solution of the Bloch equation for the complete density matrix of a many-boson system in the collective variables representation is proposed. This method allows for the effects beyond the random phase approximation. Explicit expressions for the density matrix

$$R_N(x'|x) = R_N^0(x'|x)\exp\left\{-\beta E_0+\frac{1}{2}\sum_{\mathbf{q}\neq 0}\ln\left(\frac{\alpha_q\ \tanh\left[\frac{\beta}{2}E(q)\right]}{\tanh\left[\beta\frac{\hbar^2q^2}{4m^*}\right]}\right)\right.$$
$$\left.+\sum_{\mathbf{q}\neq 0}\ln\left(\frac{1-e^{-\beta\frac{\hbar^2q^2}{2m^*}}}{1-e^{-\beta E(q)}}\right)\right\}$$
$$\times\exp\left\{-\frac{1}{4}\sum_{\mathbf{q}\neq 0}\left(\alpha_q\ \coth\left[\beta E(q)\right]-\coth\left[\beta\frac{\hbar^2q^2}{2m^*}\right]\right)(\rho_{\mathbf{q}}\rho_{-\mathbf{q}}+\rho'_{\mathbf{q}}\rho'_{-\mathbf{q}})\right.$$
$$\left.+\frac{1}{2}\sum_{\mathbf{q}\neq 0}\left(\frac{\alpha_q}{\sinh\left[\beta E(q)\right]}-\frac{1}{\sinh\left[\beta\frac{\hbar^2q^2}{2m^*}\right]}\right)\rho_{\mathbf{q}}\rho'_{-\mathbf{q}}\right\}$$

and thermodynamic functions valid in the whole temperature range are found [1]. Here, $R_N^0(x'|x)$ is the density matrix of an ideal system with an effective mass m^*, x is the set of the coordinates of N particles, E_0 is the ground-state energy, β is the inverse temperature, $E(q)=\frac{\hbar^2q^2}{2m}\alpha_q$ is the Bogoliubov spectrum, $\rho_{\mathbf{q}}=\frac{1}{\sqrt{N}}\sum_{j=1}^{N}e^{-i\mathbf{q}\mathbf{r}_j}$.

Many-particle correlations are taken into account by introducing the effective mass of an atom, which is calculated in the variational approach. The obtained analytical expressions are self-consistent in the sense that in the limit $T\to 0$ they coincide with the results by Bogoliubov, at high temperatures they provide well-known expressions of the classical many-body theory, and also reveal the phase transition connected with the Bose-condensation. Numerical computations are made using the experimental structure factor of liquid ^{4}He at $T=0$ as a source information.

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Thermodynamic analogies in economics

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The life of the people on the Earth is strongly connected with the nature of our planet, with the activity of the Sun and Space around. Two principles of being on the Earth are formulated: principle of improvement and principle of destruction.

Principle of improvement is read as: "The quality of energy, received by Earth from the Sun is higher, than the quality of energy the Earth radiates into the Space, even though the quantities of both types of energy are equal. Due to this fact the forms of being on the Earth become more and more complex and perfect".

Destruction principles says: in closed nonequilibrium system the chaos increases spontaneously. In this connection some generalized on the social systems expressions for the Free energy F and for the Inner energy E are proposed. Taking into account correlations between changing of the entropy of the system ΔS and information I given to the system accordingly $(-\Delta S) = I$, one can write the expression for the Free energy in form $\Delta F = \Delta E + TI$, where T is the temperature. When I is formulated in bytes, then dimension of T is [Energy/byte].

The energy of social system one can express in a monetary form, when introduce some monetary equivalence of energy, say, the cost of one KwH is 0,1 $. All items in formula for the Free energy can be formulated in monetary units.

In this case ΔF can express the year's achievement of the social formulation, for example gross domestic product (GDP) or gross added value and the temperature T will signify the amount of GDP done by society per one byte of information got. In such interpretation temperature T characterizes the society's perfection.

On this ground some considerations concerning circulating processes and their effectiveness are regarded. The questions about globalization processes and sustainable development are discussed.

Diffusion and stochastic particle acceleration in strong random fields

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The problem of particle acceleration and diffusion in strong random fields with well-peaked spectrum is treated analytically and numerically. The generalized Fokker-Planck equation with non-stationary velocity dependent diffusion coefficient is proposed in order to find the probability of particle transition in stochastic fields. On the basis of proposed equation mean- and mean-square velocity displacements are calculated and compared with the results of appropriate numerical simulations. It is shown that in the case of large correlation length of stochastic forces asymptotical behavior of the velocity dispersion is described by the fractional power time dependence in contrast to conventional diffusion. Qualitative dependence of the fractional exponent on the parameters of the spectrum is found. It is established that the initial stage of evolution can considerably influence the time asymptotic of the mean-square velocity displacement. The approximate analytical solution of the generalized Fokker-Planck equation is also found.

Statistical Physics 2005:

Modern Problems and New Applications

Key Note Lectures

28–30 August 2005, Lviv, Ukraine

Correlation functions of 2D and 1D electron gas

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Application of the standard rough-and-ready technique of the quantum many body theory for calculation of response and correlation functions for real Coulomb systems may result in considerable discrepancies with observable and computer simulations data. At the same time the exact asymptotic relations and sum rules for those functions and their Fourier transformations in combination with the fluctuation-dissipation theorem and casuality principle in many cases appear to be sufficient for quantitative and qualitative explanation of available experiments.

This talk is intended as an attempt to bring together those results on response and correlation functions of the electron subsystem in 1D and 2D (semi-)conductors, which can be obtained by only such tools.

Phase transitions in the coal-water-methane system

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The work is devoted to studying the system fossil coal-water-methane. The method of ^{1}H wide line nuclear magnetic resonance was used. A full ^{1}H NMR spectrum of coal-water, coal-methane, or coal-methane-water systems consists of two components: wide and narrow lines (5.5–6.5 Oe and 0.1–1.0 Oe respectively). Wide line is caused by the coal organics' hydrogen. Narrow line is contributed from the hydrogen of methane and water contained in the coal structure. The narrow line is absent in the spectra of pre-dried and degassed coal. At room temperature ^{1}H NMR lines of sorbed methane and water are very close and practically insoluble.

Nevertheless these contributions can be separated using low temperature ^{1}H NMR measurements in coal. Since sorption mechanisms of water and methane in coal are different, these species would show different behavior at lowering temperature. Mechanism of water sorption by coal is the adsorption on pores surface. On the contrary, methane sorption includes both adsorption and filling in all cavities in coal substance as in a solid solution. Phase transition (crystallization) of water occurs in the temperature range 243–173 K depending on coal carbonization and hence porous system and adsorption sites. Phase transition of methane occurs at temperatures below 90 K. Consequently, adsorbed water would crystallize during cooling much earlier than methane in water-methane mixture.

Experimental data for anthracite with $V^g = 5.0$ % are presented. Adsorbed water was crystallized from the water-methane mixture at 173 K just as in the case of artificially humidified coal. Absorbed methane is in mobile condition down to liquid nitrogen temperatures. Potential energy barrier constraining molecular movement was estimated to be about 6.6 kCal/mol for water adsorbed on anthracite, about 9.7 kCal/mol for water adsorbed on fossil coal with $V^g = 40$ %, and below 3.8 kCal/mol for absorbed methane.

It can be concluded that low temperature NMR technique allows separating contributions of absorbed water and methane in coal.

Method of intermediate problems in the theory of two-dimensional quantum dots formed by Gaussian confining potentials in the presence of a magnetic field

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It was shown that the method of intermediate problems [1], which provides convergent improvable lower bounds for eigenvalues of linear half-bound Hermitian operators in Hilbert space, can be fused with the classical Rayleigh-Ritz variational method and stochastic variational method [2] thus resulting in an efficient tool for analytical and numerical investigation with controllable or prescribed precision of the energy spectrum and eigenstates of various few-body quantum systems, among them quantum dots with small-to-medium number of excess electrons [3,4]. As an example, the energy spectrum and eigenstate problem for a 2D quantum dot formed by a Gaussian confining potential $V(r) = -V_0 \exp(-r^2/2R^2)$ was thoroughly analyzed in the presence of external magnetic field. Being smooth at the QD boundaries and of finite depth V_0 and range R, this potential can only confine a finite number of excess electrons thus forming a realistic model of a QD with smooth interface between the QD and its embedding environment. Possible generalizations of the considered model are discussed too.

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Collective excitations in a binary metallic glass Mg_{70}–Zn_{30}: A theoretical GCM study

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Collective dynamics in a glassy metallic alloy Mg_{70}-Zn_{30} is studied by molecular dynamics simulations and an analytical approach of generalized collective modes (GCM). Analytical expressions for frequencies of two branches of collective excitations in the whole region of wavenumbers are derived in a four-variable quasisolid approximation of GCM approach. In long-wavelength region these expressions correspond to bare frequencies of acoustic and optic collective excitations, and what is very important describe a crossover with increasing wavenumbers to partial behaviour of high- and low-frequency branches. In short-wavelength region the high- and low-frequency branches describe solely dynamics of light and heavy subsystems of the binary glass.

Specific ultralow-frequency collective excitations, observed as side peaks on partial and concentration dynamical structure factors in Mg_{70}-Zn_{30} are reported. The origin of the ultralow-frequency collective excitations is discussed in a connection with non-harmonic motion of particles and their jumps between different potential energy minima.

Synergetic economics of the manufacturing firm with mass production output

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Statistical Physics essntially expands the field of it's application, it penetrates into such closely-related fields of knowledge as chemistry, biology, meteorology more and more. Statistical Physics is one of the main instruments which could be useful for description of system's self-organization in the comparatively new fied of knowledge, called "Synergetic Economics". The application of the methods of Statistical Physics for it's description is possible owing to the representation of the manufacturing firm with mass production output in the capacity of the system with numerous quantity of elements (the basic products) of stochastic nature, being in the production process. Conduct of the basic products lengthwise the technological chain depends on the definite manufacturing and technological laws in accordance with the technological process of the manufacturing firm, it's production plan, the availability of manpower and equipment. The state of the production sestem's basic products at any time moment is given as the point in the two-dimensional phase space. The function of the basic product's distribution in the rate of expense's variation is set and the equation having analogy with the kinetic equation in Physics is put down here. The engineering and production function, which is analogous to the force moving the basic product lengthwise the technological chain of the production process, is given and can be determined with the help of technical documentation of the article's manufacture approved in the manufacturing firm. The generating function describing the interaction of the basic products (the system's elements) during their moving lengthwise the technological chain of production process with technical equipment, is based on the equipment disposition schemes and it's technical characteristies according to the schedule of the workpieces machining. The closed system of balances equations for the moments of distribution function is put down here in the zero approximation with the small parameter, with the usage of the kinetic equation. The system of balances equations describes the conduct of the basic economical macroscopic rates of the production system, such as process stocks, pase and dispertion of the production output lengthwise the technological chain. With the help of the balances equations the well-known relations of the business operation theory used for the calculation of stocks and pase of the production output were obtained.

A microscopic theory of photonucleation: Density functional approach for the properties of a fluid of two-level atoms, a part of which is excited

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We use the density functional approach to examine the properties of the nonuniform (two-phase) fluid of two-level atoms, a part of which is excited. From the analysis of the equation of state of a gas of two-level atoms, a part of which is excited, (see [1–4]) the following density functional of the grand thermodynamical potential emerges

$$\Omega[\rho(\mathbf{r})] = \Omega_{\rm CS}[\rho(\mathbf{r})] - \frac{6\sigma^3 a(c_1,T)}{\pi}\int_{|\mathbf{r}_1-\mathbf{r}_2|\geq 2\sigma} {\rm d}\mathbf{r}_1{\rm d}\mathbf{r}_2 \frac{\rho(\mathbf{r}_1)\rho(\mathbf{r}_2)}{|\mathbf{r}_1-\mathbf{r}_2|^6},$$

$$a(c_1,T) = \frac{1}{32}a^2 v(E_1-E_0)\left(c_0-c_1+2c_0c_1\frac{E_1-E_0}{kT}\right).$$

Here $\Omega_{\rm CS}[\rho(\mathbf{r})]$ is the density functional of the grand thermodynamical potential of hard spheres within the Carnahan-Starling approximation, σ is the atom radius, $v=(4\pi\sigma^3)/3$, c_1 is the concentration of excited atoms, $c_0+c_1=1$, E_1-E_0 is the excitation energy. We use this expression to calculate the nucleation barrier for the vapour-to-liquid phase transition [5] in the presence of excited atoms.

Further details can be found in [6].

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Diamagnetism of electron gas

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It is well known that many metals are diamagnetic. The diamagnetism of an electron gas seems to be a consequence of the dynamics of a single classical particle. However, the application of classical statistical mechanics to the theory of the electron gas given in the works by N. Bohr and J. H. van-Leeuwen has led to the zero value of the magnetic moment.

It is generally agreed that the diamagnetism of the electron gas has been explained as a quantum effect by L. D. Landau. But it can be shown that appearance of the diamagnetism in the Landau's work is a result of a mistake. L.D. Landau neglects the orbit dimension, which determines the energy dependence of the degeneration of an energy level. The approximate degeneration is then used to compute the thermodynamic potential. This results in a loss of a term which is small compared to the main term, however, in distinction to the latter, it depends on the magnetic field and, therefore, contributes to the magnetic moment. A consistent computation of this contribution shows that it is paramagnetic and several hundred times greater than the diamagnetic moment computed by Landau.

In the above works the computations were performed with the distribution density that depends on the system Hamiltonian and volume bounded by an impenetrable wall. According to the principle offered by A. Ya. Khinchin, the distribution density must depend on those integrals of motion and external parameters, which determine the bounded domain in the phase space, within which the phase trajectory of the chaotic motion of the system remains for a indefinitely long time. We consider a two-dimensional gas of charged particles, confined by the magnetic field, as an example. For this case, it is shown that the Hamiltonian and a linear combination of the Hamiltonian and the angular momentum are the integrals of motion of the system,which bound a domain in the phase space. The computation of the average magnetic moment using a distribution density depending on these integrals of motion results in the diamagnetism.

Are public transport networks scale-free?

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Public transport (PT) networks are defined as sets of public transport routes and stations serviced by these routes. These networks are generally assumed not to possess a power-law scaling in their node degree distributions. Only recently, in the analysis of very large networks such scaling behaviour was observed [1] and a conjecture about scale-free properties of PT networks was formulated. However, these conclusions are based on statistics of the networks of three cities only and are to be considered as preliminary ones. Our present study extends the statistics, analyzing public transport networks of up to 20 major cities with typical number of routes/stations ranging from 68/573 (Kyoto) to 1883/19284 (Los Angeles). We find evidence of scale-free behaviour of different quantities characterizing PT networks.

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Superflow of electron-hole pairs in quantum Hall bilayers: The role of interlayer tunneling

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The possibility of superfluidity of electron-hole pairs in bilayer electron systems was predicted many years ago. Later, it was understood that the most promising systems for a realization of that effect are electron-electron bilayers subjected by a strong perpendicular to the layer magnetic field. At total Landau level filling factor close to unity the spontaneous interlayer phase coherence emerges in such systems. In particular, it should manifest itself in a counterflow superfluidity and Josephson-like tunnel conductivity. Recent experimental observation of these features is considered as a strong evidence for the excitonic superfluidity in quantum Hall bilayers.

In this report we study the effect of tunneling on the supercurrent states in bilayer systems with pairing of electrons and holes of adjacent layers. We obtain the system of equations for the phase and the modulus of the order parameter that describes the electron-hole pairing in bilayers with the interlayer tunneling. The system of equations derived allows to visualize the transformation of the normal current to the supercurrent at the edges of the bilayer system. It is shown that the space distribution of the supercurrent depends on the values of the income and outcome currents at the edges as well as on the ratio between the Josephson length and the linear size of the sample. For the counterflow setup, we find that two supercurrent states can be realized: the single kink state and the multiple Josephson vortex state. The kink state emerges at low current at one edge of the sample and in such a state the current does not reach the other edge (if the length of the sample exceeds the Josephson length). If the current at the one edge is larger than the critical one (which we call the lower critical current), the multiple Josephson vortex state is formed and the current reaches the other edge of the sample.

On the rigorous derivation of kinetic equations

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We argue possible approaches to the problem of the rigorous derivation of kinetic equations from underlying many-particle dynamics.

As it is known, the evolution of states of infinitely many particles is generally described by sequences of n-particle distribution functions which are solutions of the initial value problem to the BBGKY hierarchy of equations. Recently [1,2] new methods of the construction of solutions of the initial value problem to the BBGKY hierarchy have been developed. In particular, the rigorous description of microscopic dynamics of a hard sphere system has been given and the Boltzmann-Grad limit theorem has been proven [1].

In scaling limits the evolution of states of infinite particle systems can be effectively described by the one-particle distribution function which satisfies the kinetic equations.

We demonstrate that in fact, if initial data are completely defined by the one-particle distribution function then all possible states of infinite particle systems at arbitrary moment of time can be described only within the framework of the one-particle distribution function without any approximations.

In suitable functional spaces for the initial data, for instance, initial data satisfying the “chaos” property [1], we prove that the Cauchy problem to the BBGKY hierarchy is equivalence to the corresponding initial value problem for certain generalized kinetic equation and an infinite sequence of explicitly defined functionals depending from the solution of this generalized kinetic equation. We note, that the specific kinetic equations can be derived from constructed generalized kinetic equation in the appropriate scaling limits.

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Magnetocaloric effect in frustrated spin systems

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Due to the magnetocaloric effect, adiabatic changes of the magnetic field applied to a magnet yield a change of temperature. We discuss recent theoretical results for the magnetocaloric effect in the vicinity of field-induced quantum phase transitions in quantum spin systems. Geometrically frustrated magnets are of special interest since they exhibit large entropies at low temperatures, promising a large magnetocaloric effect. A comparative theoretical study of different one-dimensional quantum magnets has shown that lower temperatures can indeed be achieved by adiabatic (de)magnetization of a frustrated system. Here we present new results on higher-dimensional lattices. For example, on the kagomé lattice, we find a large number of zero- and low-energy excitations, giving rise to an enhanced magnetocaloric effect. These results suggest applications of frustrated quantum magnets e.g. on kagomé- and pyrochlore-type lattices for efficient low-temperature magnetic refrigeration.

Reentrant transitions of a mixed spin-1/2 and spin-1 Ising model on the diced lattice

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Magnetic behavior of the mixed spin-1/2 and spin-1 Ising model on the diced lattice is studied by the use of an exact star-triangle mapping transformation. It is found that the uniaxial as well as biaxial single-ion anisotropy acting on the spin-1 atoms potentially cause a reentrant transition with two consecutive critical points. Contrary to this, the effect of next-nearest-neighbor interaction between the spin-1/2 atoms possibly leads to a reentrant transition with three critical temperatures in addition to the one with two critical points only. The shape of the total magnetization vs. temperature dependence is particularly investigated for the case of ferrimagnetically ordered system.

Non-Gaussian fixed points in the method of I.R. Yukhnovskii

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A mathematical formalization of the method developed by I.R. Yukhnovskii [1] has been elaborated. This formalization gives a possibility to extend the method to other classical models manifesting critical behavior, as well as to the quantum case. In its framework, the sequence of partially integrated partition functions is represented by a sequence of functions with prescribed analytic properties, defined on a complex Hilbert space (the complex plane in the simplest case). These sequences are generated by a nonlinear integral transformation defined on the corresponding topological spaces. The non-Gaussian fixed points of this transformation are obtained as solutions of certain nonlinear differential equations. Their analysis has been performed and the physical consequences have been discussed.

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Light scattering studies on the particles with permanent and induced dipole moments in solutions

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The intensity, polarization and spectral distribution of the scattered light convey significant information about processes that occur in the liquid. Further information on the processes can be obtained by studying the liquid which is subjected to different fields. Such fields cause splittings, shifts and spectrum line deformations to appear. The applying of external fields changes the feature of Brownian motion and provides control over the changes in experimental spectra.

We investigate theoretically Rayleigh scattering of light by a suspension of anisotropic ellipsoidal particles subjected to external fields. The charges and dipole moments of most protain molecules are so large that even for low concentration, the average energy of the interaction between them is comparable with kT. This fact has to be taken into account when developing the Brownian motion theory for such systems.

We will consider the dynamics of Brownian rigid macromolecules dissolved in dielectric fluid and subjected to external fields. An external electric field polarizes the particles. The oriented dipoles interact with one another. Both induced and permanent dipole moments of particles are included. A dipole-dipole interaction of the density fluctuations develops.

It is shown that the action of the external fields induces deformations in the shape of scattering line and results into the non-monotonic frequency dependence of spectral lines of depolarized scattering with additional local maxima in the spectra.

Statistical physics of model system with interaction

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The unified approach to description of model system interacting particle is proposed. Based on statistical approach is described possible formation of spatially inhomogeneous distribution in the system of interacting particles. The condition of cluster's formation both in gas and condensed phases was obtained in this system. Is studied the dynamics of cluster's formation in system of interacting particle. Is described the cluster-formation processes in the system with short-range and long-range interaction. A procedure is proposed for selecting the probable states whose contribution in the thermodynamic behaviour of the system is dominant. This technique makes it possible to take into account fluctuation of any scales and to obtain a closed expression for the parameters of the new phase formation, in particular its dimensions, lifetime, and time of relaxation towards a thermodynamically stable state. The feasibility of experimental observation of the new phase bubble parameters' dependence on the governing quantities is discussed.

The joint Rouse-Zimm theory of the dynamics of polymers in solutions

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The Rouse (R) and Zimm (Z) models have been proven as successful models in describing the universal properties of polymers. In spite of this, a number of questions remains unsolved. Some problems could be due to an improper use of these theories. We show that the "joint" R–Z theory, in which the Z and R models are just limiting cases of infinitely large and small draining parameter, should be used in the description of the polymer dynamics. We propose the R–Z theory of the dynamics of polymers in dilute solution. The equation for the position vectors of the beads of the chosen "test" polymer is built. The equation of motion for the bead is solved together with the hydrodynamic equations for the solvent velocity that take into account the presence of other polymer coils in solution as the obstacles to the solvent flow. By preaveraging the Oseen tensor the equation for the polymer normal modes is obtained and the relevant time correlation functions are found. As distinct from the situation of a single polymer in the solution, the solvent flow is disturbed by other coils and with growing concentration c it "freezes", which indicates the tendency to hydrodynamic screening. We consider the concentration effect on the diffusion of the polymer as a whole as well as on the relaxation of its internal modes. The coil diffusion coefficient has the form $D(c) = D_Z(c) + D_R$ and the relaxation rates of the internal modes $p = 1, 2, \ldots$ are $\tau_p^{-1}(c) = \tau_{pZ}^{-1}(c) + \tau_{pR}^{-1}$, with the R contributions being independent on c. Analytical expressions are obtained for both $D(c)$ and $\tau_p(c)$. When c increases, the Z contributions to $D(c)$ and $1/\tau_p(c)$ decrease and show a transition to the Rouse behavior of the polymer. Since an isolated polymer always changes its dynamics in the time from the R- to Z-type behavior, this transition should be viewed as a concentration- and time-dependent process. With the aim to interpret experiments, the dynamic structure factor of the polymer, the relaxation modulus, and the shear viscosity of the solution have been calculated.

Extreme emulsification: Formation and structure of nanoemulsions

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Nanoemulsions are dispersions of nanoscale droplets of one liquid in another immiscible liquid and are stabilized against coalescence by a surfactant. We examine the production of silicone oil-in-water nanoemulsions by a high-pressure microfluidic device over a wide range of droplet volume fractions, ϕ, and sodium dodecylsulfate surfactant concentration. By monitoring the droplet size distribution using dynamic light scattering, we show that nanoemulsions having droplet diameters down to 30 nm can be produced at shear rates exceeding $10^8 s^{-1}$. Moreover, we show that shear-induced coalescence can become an important factor as ϕ approaches the random jamming limit of spheres at $\phi_{\mathrm{MRJ}} = 0.64$. Due to the extremely large Laplace pressures inside the droplets, nanoemulsions made using low molecular weight silicone oil droplets coarsen (i.e. grow) rapidly through Ostwald ripening following emulsification. However, nanoemulsions made using high molecular weight silicone oils do not evolve significantly over time scales of many months, due to the lower solubility of the oil in the aqueous phase. By diluting and ultracentrifuging these nanodroplets, we can fractionate them to make them highly monodisperse in size. The resulting concentrated nanoemulsions are highly elastic and appear transparent, since the droplets are much smaller than the wavelength of visible light. We use small angle neutron scattering to investigate the static structure of monodisperse nanoemulsions from the dilute to the concentrated limit in ϕ. We find that a nearest neighbor peak develops in the structure factor as we increase ϕ, yet, by contrast to hard spheres, the peak subsequently decreases as we approach the random jamming limit. This unusual behavior may indicate that the deformability of the droplets is facilitating a higher degree of quenched-in disorder when ϕ is rapidly raised.

Effective temperature of self-similar time series

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The work is devoted to both analytical and numerical studies of self-similar time series. We start analytical consideration with elaboration of a model which allows us to address a time series as slightly non-extensive thermodynamic system, whose entropy and internal energy are calculated. Moreover, thermodynamic-type characteristics such as temperature, volume, pressure and free energy are introduced. Their testing for the model of ideal gas is shown to be basis for statistics of self-similar time series. Corrections to the ideal gas approach are calculated when external field and particle interaction are taken into account. On the basis of Van der Waals model, we obtain the expressions for the specific heat and susceptibility as functions of the temperature. The physical meaning of the results obtained is discussed within the framework where the predictability of behavior of time series is mimicked as stability conditions of a non-ideal gas. We find maximal magnitudes for time interval and minimal resolution scale of the value under consideration. It is shown that a temperature governing time series statistics is exponential measure of a self-similarity index related to fractal dimension of the time series.

Testing of the analytical consideration is based on numerical scheme of non-extensive random walk, whose stochastic equation and its solutions are treated. As a result, we obtain non-trivial time series, whose form is governed by a friction coefficient fixing related fractal dimension.We introduce a statistical scheme that allows us to consider modeled time series as a grand canonical ensemble, for which we calculate entropy and internal energy as functions of particle number. Then, we find numerically effective temperature and show that its value is reduced to averaged kinetic energy per one particle of ideal gas. Finally, we confirm numerically exponential dependence of the effective temperature on the fractal dimension that was found analytically. We discuss also multifractional and clustering properties of time series.

XY spin fluids in an external magnetic field: an integral equation approach

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A method of integral equations is developed to investigate anisotropic fluids with planar spins in the presence of an external magnetic field. As a result, the calculations for these orientationally ordered systems appear to be no more difficult than those for an isotropic mixture of simple homogeneous fluids. The method is applied to ferromagnetic XY spin fluid models in an external field to study phase coexistence properties. The soft mean spherical approximation is employed for the closure to the anisotropic Ornstein-Zernike equation. The Born-Green-Yvon and Lovett-Mou-Buff-Wertheim equations are used to describe the orientational distributions. The phase diagrams are obtained in the whole range of varying the external field for a wide class of XY spin fluid models with various ratios for the strength of magnetic to nonmagnetic Yukawa-like interactions. Different types of the phase diagram topology were identified. They are classified by the existence of critical, tricritical or critical end, and triple points, related to transitions between gas, liquid, para- and ferro-magnetic states, accompanied by different external field dependencies of the gas-liquid and liquid-liquid critical temperatures and densities. Detailed comparisons with Gibbs ensemble and multiple-histogram reweighting Monte Carlo simulations have shown that the proposed approach is powerful enough to give a quantitative description of phase transitions in the XY spin fluid systems.

This work was supported by the Austrian Fonds zur Förderung der wissenschaftlichen Forschung, project No P15247.

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Charge-charge correlations near gas-liquid critical point

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For the last decade, both the phase diagrams and the critical behavior of ionic fluids have been intensively studied using experimental, theoretical as well as computer simulation methods. Nevertheless, in spite of significant progress in this field, understanding of ionic systems is far from complete.

In this report we address a relevant issue that concerns the behaviour of the two-point charge-charge correlation function near the gas-liquid critical point (CP) where the density fluctuations diverge strongly. Recently Aqua and Fisher [Aqua J.N. and Fisher M.E. 2004 Phys. Rev. Lett., **92** 135702] studied this issue using multi-component lattice gas generalization of the spherical model. For a non-symmetrical model they found that the Stillinger-Lovett (SL) rule fails at the CP.

In the present work we consider a charge- and size-asymmetric continuous model of an ionic fluid. In the random phase approximation we obtain the explicit expressions for the density-density, charge-charge and charge-density correlation functions valid far and close to the gas-liquid CP. The results obtained for the charge-charge correlation function demonstrate that the second-moment SL rule is satisfied away from the CP but not, in general, at the CP. Some generalizations of these results for the case, when the fluctuations are taken into consideration, are discussed.

Generalized Gross-Pitaevskii equations for $T \neq 0$ with taking into account binary correlations of the Bose condensate particles

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In our paper (S.Peletminskii, A.Sokolovsky) kinetics of the weak interacting Bose-gas in the presence of Bogolyubov condensate was built with the wave function of the condensate $\psi(x,t)$ and the Wigner distribution functions of the Bogolyubov quasiparticles $\mathrm{f_p}(x,t)$ as RD parameters. On the base of these kinetic equations with the help of the Chapman-Enskog method the next stage of the evolution of the system was investigated at which quasiparticles are in equilibrium with spatially uniform temperature $T(t)$ and drift velocity $\omega_n(t)$. A system of equations for variables $\psi(x,t)$, $T(t)$, $\omega_n(t)$ was obtained that is our generalized Gross-Pitaevskii equations for $T \neq 0$. The next stage of the present work is to include in the set of RD parameters not only wave function of the condensate particles $\psi(x,t) \equiv \overline{\psi(x)}^t$ but the wave function of the pairs $\overline{\psi(x)\psi(x')}^t$ also. It will correspond to the real situation according to which the condensate is a mixture of condensed particles and pairs of particles. The mentioned RD was built on the base of idea: the RD theory without nonequilibrium correlations as independent RD parameters but with a random initial state leads with the help of the corresponding averaging to the RD theory taking into account nonequilibrium correlations (S.Peletminskii, A.Sokolovsky, Yu.Slyusarenko). This idea gives the following system of equations for RD parameters $\eta_a(t)$ (i.e. for $\psi, T, \vec{\omega}$) and for the corresponding binary correlations $g_{aa'}(t)$

$$\partial_t \eta_a = e^{A(g)} L_a(\eta), \partial_t g_{aa'} = e^{A(g)} \sum_{a''} \left(g_{aa''} \frac{\partial L_{a'}(\eta)}{\partial \eta_{a''}} + \left(a \leftrightarrow a'\right) \right)$$

$(A(g) \equiv \frac{1}{2} \sum_{aa'} g_{aa'} \frac{\partial^2}{\partial \eta_a \partial \eta_{a'}})$. For our purposes it is enough to include in the set of correlations $g_{aa'}$ correlation between $\psi(x,t)$ and $\psi(x',t)$.

This work was supported by SFFR of Ukraine (project No. 2.7/418) and in part by INTAS (project No. 00-577).

The geometric representations in classical and statistical equilibrium thermodynamics (contact, Riemann and information geometries)

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By the aid of the formalism of the differential 1- and 2-forms in the framework of the contact geometry the analysis is given of the family of r-dimensional Gibbs surfaces $G^{(r)}$, parametrized by the Euclidean r-dimensional ($r \geq 2$) base space $R^{(r)}$ of the thermodynamical parameters for the macroscopic system in the state of thermal equilibrium. It is shown, that $G^{(r)} = L^{(r)}$, where $L^{(r)}$ is the family of Legendre (sub)manifolds, which describe the solutions of the Pfaff equations (up to contactomorphisms) in the Euclidean space $R^{(2r+1)}$; Darboux theorem in this case corresponds to the thermodynamic Gibbs-Helmholtz relations.

In the scope of the classical thermodynamics (CTD) the surfaces $G^{(r)}$ are considered at first as imbedded in $R^{(r+1)}$ Riemannian manifolds. It is shown, that the conditions of the thermodynamic stability of the system (in the form of Gibbs inequalities) imposed by the Second Law relative to spontaneous equilibrium fluctuations demand all the $G^{(r)}$'s to be strictly convex. This, in turn, means the strict positivity of the external Gauss curvature K, which is proportional to $\mathrm{Det}\, h$, where h is the Hessian of the Massieu-Planck potential for the system under consideration.

Alternatively, $G^{(r)}$ are considered as Riemannian manifolds without any imbedding, but with h chosen as the metric matrix g. We consider the most interesting case $r = 2$, which is not subjected to the restrictions of the Liouville theorem and allows a great variety of conformal, or "isothermic" base space coordinate transformations. In this case the Gauss' "theorema egregium" expresses K (now as the internal curvature) through the derivatives of g, and in this way we obtain some conditions of the thermodynamic stability additional to the standard conditions which include only the positive definiteness of matrix h.

In the framework of the statistical thermodynamics (STD) the information geometry, or geometrostatistics (the last term is due to Kolmogorov) is studied using the fact that the global quasi-metric in the topological space P of all parametric r-dimensional ($r \geq 2$) probability

density functions (pdf) is locally equivalent to the Riemannian metric with the metric matrix equal to the Fisher information matrix g^{F}, which is (by definition) always positive definite.

In the case of strictly additive base space variables due to the theorem of Koopman-Pitman-Dynkin-Jeffries P is the space of all exponential pdf, which were obtained in STD much earlier and are known as Gibbs-Einstein-Szilard pdf. For this class of pdf it is shown that g^{F} equals to h and therefore the Fisher-Kramer-Rao theorem implies Einstein thermodynamic "uncertainties relation". Moreover, the space P, considered as the embedded Riemannian manifold parametrized by the base space $R^{(r)}$, should be, just as $G^{(r)}$, be strictly convex, because in this case g^{F} equals to g. Finally, the expressions are obtained for g^{F} and K (at $r = 2$) for the q-deformed Gibbs-Einstein-Szilard pdf, i.e. non-exponential pdf of the Renyi-Tsallis type.

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Dynamical cluster studies of nonresonant Raman scattering in the Falicov-Kimball model

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Recently we proposed the Dynamical mean field theory (DMFT) solution for electronic Raman scattering in the Falicov-Kimball model which is widely used to describe strongly correlated materials. Within this approach we have shown the existence of isosbestic point and the importance of resonant effects that may dramatically enhance non-resonant features in Raman spectra [1].

However DMFT, which is exact in infinite dimensions, is not good enough to describe the one and two dimensional cases. On the other hand, it is important to check whether the features we obtained in Raman spectra will survive in low dimensions. Therefore we employ recently developed Dynamical cluster approximation (DCA) technique to solve for non-resonant electronic Raman scattering in two-dimensional Falicov-Kimball model.

We investigate non-resonant Raman spectra for different scattering geometries and optical conductivity at half filling on both sides of metal-insulator transition. The spectra exhibit more complex structure with the increase of cluster size yet isosbestic point survives.

1. Shvaika A.M., Vorobyov O., Freericks J.K., Devereaux T.P., Phys. Rev. Lett. **93**, 137402 (2004); Phys. Rev. B **71**, 045120 (2005).

Conductivity of metallic hydrogen

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We calculate the electroresisitvity of metal hydrogen within the framework of pertubation theory in electron-proton interaction. To this end we employ the Kubo linear response theory while using the two-time retarded Green functions method to calculate the relaxation time. The expressions for the second and third order contributions are given. To describe the electron subsystem the random phase approximation is used, allowing for the exchange interactions and correlations in a local field approximation. Two-particles structure factor of the proton subsystem is assumed to be given by the Percus-Yevick equation in hard sphere approximation. An effective hard sphere diameter and the packing fraction are the only parameters of the theory in this case. They depend on the density and the temperature of metallic hydrogen. Settin the hard sphere diameter equal to the ionic radius of hydrogen, and using the typical values of the packing fraction for alkali metals, we obtain for the second and the third order contributions the valus 53 microOm*cm and 23 microOm*cm correspondingly. The dependence of the second and the third order contributions on the parameters of the theory is investigated. It turns out that both the second and the third order contributions decrease with increase of the dinsity and the temperature of metal hydrogen, at that the second order contribution exhibis more rapid decay.

Structural interactions and “softness” of the matter

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When two mesoparticles are suspended in a fluid medium, besides their direct interaction, they experience an extra force that is mediated by the suspending medium. In the case when medium is an aqueous solution, this extra force is usually referred to as the hydration force. For the case of a more complex suspending medium (such as macroion or nanocolloidal suspensions, etc.), the forces induced by the background fluid would be better referred to as *structural forces*, since these forces originate from the changes in the local structure of the suspending medium. The manifestation of structural changes is associated with the phenomenon of layering or stratification of the species of the suspending fluid next to the confining surfaces. When the separation between surfaces is commensurate with integral number of fluid layers - then the pressure inside the gap between surfaces is increased. Otherwise, if the separation between surfaces is smaller (or larger) than it is necessary to accommodate an integral number of suspending fluid layers - then the pressure is decreased, indicating a repulsive or attractive force that is exerted by the confined fluid on the confining bodies. In this lecture we show that the conditions of the appearance and existence of the structural forces are equivalent to the definition of the soft matter systems. Some important properties of the selected soft matter systems governed by structural interactions are discussed.

Equilibrium and diffusion properties of lattice gas systems

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Lattice gases (LGs) are extensively used to model equilibrium and non-equilibrium properties of liquid-like subsystems in solids or on their surfaces including solid electrolytes, semiconductors, metals, intercalation compounds and many others. For analytical calculations of equilibrium thermodynamic and structural properties of LGs with interparticle interactions the self-consistent diagram (SCDA) and diagram (DA) approximations were suggested. The DA is as almost simple as the quasi-chemical approximation and as almost precise as the SCDA.

Different properties are investigated for several LG models. The chemical potential vs concentration dependence allows one to investigate phase transitions. The thermodynamic factor that is inversely proportional to the mean square concentration fluctuations is calculated. This factor is of great importance because it connects the chemical diffusion coefficient that enters the first Fick's law and the kinetic diffusion coefficient, the latter being the Onsager coefficient. The chemical capacitance is inversely proportional to the thermodynamic factor. Structural properties are represented by distribution functions and order parameters.

Contrary to Hamiltonian systems LG dynamics is described by the irreversible master equation of the Kolmogorov type. A Mori-type equation for the lattice concentration is constructed and the general expression for the diffusion coefficients is developed. In contrast to systems with reversible dynamics the relevant or quasiequilibrium distribution significantly contributes to the diffusion coefficients.

Extensive analytical and Monte-Carlo simulations were performed for different LG models. In the case of LG with nearest neighbor attractive interactions the static contribution describes the diffusion coefficients with high accuracy that means the memory effects are of minor importance. However, for repulsive interactions in the range where the ordered phase exists the memory effects are important.

Many interesting phenomena are attributed to two-component LGs. When concentration of less mobile particles is around of 0.5 or higher they force the faster particles to reduce mobility to their level. This behavior is observed for attractive as well as repulsive interactions.

Lattice dynamics and phase transitions in $Sn_2P_2S(Se)_6$ ferroelectrics

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A lattice dynamics of $Sn_2P_2S_6$ and $Sn_2P_2Se_6$ crystals and their solid solutions was analyzed in a polarized ions model with fitting of calculated phonon spectra to light and neutron scattering data. An instability of a lowest frequency polar optical Bu mode of a paraelectric phase $P2_1/c$ could be modeled by recharging between cations Sn and chalcogen atoms S(Se), and by changing of the chalcogen atoms polarizability. In a ferroelectric phase Pc the soft mode is stabilized by shifting of the tin atoms, which contributes to rise of spontaneous polarization, and by partial opposite recharging.

The soft optical branch of the paraelectric phase of $Sn_2P_2S_6$ has a minimum at a Brillouin zone (BZ) center what is connected with second order transition to the ferroelectric phase. In the paraelectric phase of $Sn_2P_2Se_6$ such branch has the minimum near the BZ center. Here a condensation of mixed soft optic and acoustic branches occurs at a continuous transition to an incommensurate phase. This difference has origin in more strong long range dipole-dipole interaction for $Sn_2P_2S_6$ — bigger effective charges of ions determine stronger LO-TO splitting of the soft mode. A two-mode concentration transformation of the soft branch in solid solutions is expected and could be considered as origin of nonergodic effects near a Lifshitz point which divides transitions into ferroelectric and incommensurate phases with a spontaneous polarization and modulation vectors placed in a monoclinic plane.

Statistical Physics 2005:

Modern Problems and New Applications

Short Communications

28–30 August 2005, Lviv, Ukraine

Nonlinear effects in the regularity problems for infinite dimensional evolutions of classical Gibbs models

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We discuss regularity properties of evolutions of the classical lattice Gibbs systems. Such models are important because they give lattice approximations of the Euclidean field models in high dimensions with nonlinear potential interaction.

We obtain information about C^∞ regularity properties of their heat dynamics. The main attention is devoted to the influence of nonlinear interaction and infinite dimensionality on the topologies of spaces of continuously differentiable functions, that are preserved under the action of semigroup.

The suggested approach is based on a new type nonlinear estimates on the high order variations of corresponding heat diffusion equations. We also demonstrate how one can work with regularity problems in case of nonlinear differential equation, i.e. when the classical Cauchy-Liouville-Picard regularity scheme, initially developed for quasi-linear and Lipschitz equations, does not work.

Free energy landscapes for dimerization of amyloidogenic tetrapeptides

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The oligomerization of four peptide sequences, KFFE, KVVE, KLLE and KAAE is studied using replica exchange molecular dynamics simulations with an atomically detailed peptide model. Previous experimental studies by Tjernberg and co-workers [J. Biol.Chem., 277 (2002) 43243] reported that of these four peptides, only those containing phenylalanine and valine residues form fibrils. We show that the fibrillogenic propensities of these peptides can be rationalized in terms of the equilibrium thermodynamics of their early oligomers. Thermodynamic stability of dimers, as measured by the temperature of monomer association, was seen to be higher for those peptides that are able to form fibrils. While the relative high and low stabilities of the KFFE and KAAE dimers arise from their respective high and low inter-peptide interaction energies, the higher stability of the KVVE dimer over the KLLE system results from the smaller loss of configurational entropy accompanying the dimerization of KVVE. Free energy landscapes for dimerization are found to be strongly sequence-dependent, with a high free energy barrier separating the monomeric and dimeric states for KVVE, KLLE and KAAE sequences. In contrast, the most fibrillogenic peptide, KFFE, displayed downhill assembly, indicating enhanced kinetic accessibility of its dimeric states. The dimeric phase for all peptide sequences is found to be heterogeneous, containing both anti-parallel beta-sheet structures that can grow into full fibrils as well as disordered dimers acting as on- or off-pathway intermediates for fibrillation.

Collective behavior of self-propelling particles in a circle with reflecting boundary conditions

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We study the collective behavior in the system of SPP (self-propelling particles) with nonholonomic constraints imposed on their velocities known as Czirok-Vicsek automaton or algorithm (CVA) in 2D. The kinetics of the transition to the state of ordered motion is investigated under different boundary conditions and noise intensity. The results are interpreted within simple relaxation model of the form

$$\varphi(t) = \varphi_\infty(1 - \exp[-t/\tau]),$$

where φ is the corresponding order parameter. The modified CVA is considered where the velocity distribution is introduced. The behavior of such modified model is compared to that of the CVA with noise. The equilibrium profiles for the particle density and velocities are compared. The dependence of the relaxation time τ on the relevant parameter is discussed.

Multilevel simulations of macromolecules

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Macroscopic properties of materials are sensitive to details of interaction on the molecular scale. Computer simulations is a powerful tool for studying the connection between macroscopic and microscopic levels, but if very-large-scale features need to be sampled, they suffer from a slowing-down due to locality of common numerical processes. Macromolecules possess the large spectrum of length scales characterizing molecular structure; therefore a new computational methodology should be developed for successful investigations of such systems.

Systematic Upscaling (SU) is a new general approach for studying many-body problems. It is based on local processing and repeated coarsening, creating increasingly coarser description (in terms of coarse-level variables) of the same physical system. A coarse-level description is constructed from a current level in accordance with some general principles.

The Multilevel Monte Carlo algorithm for simulations of macromolecules is developed using SU. In order to perform common Monte Carlo local processing at each level, a Hamiltonian-like functional of coarse variables is constructed. The method is applied for simulations of a single polymer chain with finitely extensible non-linear elastic model of interactions. Possible sets of coarse variables are analyzed and numerical results for the temperature dependence of probability distributions of end-to-end distances are presented.

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Thermal motion in normal and supercooled water according to data of quasi-elastic incoherent neutron scattering

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In the present work the following important problems are investigated:

1) the value and temperature dependencies of the self-diffusion coefficient, its one-particle and collective parts;

2) the value and temperature dependence of the residence time for molecular thermal motion;

3) the temperature interval, where structural, thermodynamic and kinetic properties of water are determined by the H-bond subsystem.

For the solution of the first two problems the wave vector dependence of the half-width for incoherent neutron scattering peak is analyzed in details. It is shown that the applicability region of the diffusion approximation is limited by the interval $0 \leq \vec{k}^2 < 0.7\text{Å}^{-2}$. The usage of experimental points from the larger wave vector interval leads to considerable errors in the values of enumerated above parameters. It is establish that the quasi crystal-like character of thermal motion in supercooled region and normal states of water takes place only up to temperature $T_* \sim 320$ K. The similar estimate for T_* is also obtained from the comparative analysis of the temperature dependencies of the shear viscosities for water and argon. It is shown that the averaged number of H-bonds per molecule at $T > T_*$ becomes less than two. So the three-dimensional H-bond network exits in water only at lower temperatures.

Origin and applications of fractional kinetic equations

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Recently, fractional kinetic equations of the diffusion, diffusion-advection, and Fokker-Planck type were recognized as a useful approach for the description of transport dynamics in complex systems. The talks presents a short review on the origin, properties and applications of fractional kinetics. Namely, the relation to the random walk schemes is discussed, the properties of the solutions are visualized, and the applications to a few systems ranging from the iterated maps to polymers are demonstrated. The fractional kinetic equations are applied to describe non-Gaussian Levy processes in external potential fields, and non-trivial relaxation phenomena as well as non-Boltzmann stationarities. Also, a new class of generalized diffusion equations with time and space fractional derivatives of the distributed and variable orders is proposed for the kinetic description of anomalous diffusion and relaxation phenomena, whose diffusion exponents vary with time and which, correspondingly, cannot be viewed as fractal (self-affine) random processes possessing a unique Hurst exponent.

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Primitive model for cation hydrolysis: A molecular dynamics study

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A model of primitive cation M^{Z+} in water is introduced in order to clarify the influence of ion charge on hydration structure and dynamic properties of highly charged cations in aqueous solutions. A flexible non-constrained model for water molecules is used. The considered model in the case of monovalent cation M^+ reduces to the realistic model for hydration structure of Na^+. It is shown that for divalent ion M^{2+} the strong cation-water electrostatic interaction leads to formation of stable structures constituted by six water molecules octahedrally arranged around the cation. The cation-oxygen attraction and cation-hydrogen repulsion modifies the octahedral hydration configuration of model cations M^{3+} and M^{4+} and additional water molecules can join the hydration shell. The increase of cation charge results in increase of O–H bond length of water molecules in cation hydration shell. Further increase of ion-water electrostatic interaction causes the loss of some protons from hydration shell of cations M^{4+} and M^{5+}, that is interpreted as a cation hydrolysis effect. For correct description of this phenomenon the considered model is improved by modelling the effects of charge redistribution between hydrolysis products, which essentially modified and stabilized the hydrated-hydrolyzed structure of cation. The influence of cation charge on dynamical properties of cation M^{Z+} and oxygens in its hydration shell were investigated and analyzed.

Phase behavior of Ising mixtures

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The mean field theory for the pure Ising fluid was recently extended to binary mixtures of an Ising and a van der Waals fluid (*Ising mixtures*) [1,2]. Depending on three parameters describing the relative magnetic and nonmagnetic interaction strengths, the theory predicts a rich multicritical behavior in the three dimensional x, T, p-phase diagrams, featuring tricritical consolute and plait point lines, lines of critical end points and magnetic consolute point lines. In order to ascertain if the predicted topologies are also found in the presence of fluctuations we have performed extensive Monte Carlo (MC) [2] as well as integral equation (IE) calculations, investigating both first order (liquid-vapor and demixing) and second order (paramagnetic-ferromagnetic) phase transitions for mixtures of a Lennard-Jones fluid and a Lennard-Jones-Yukawa Ising fluid. The simulation methods we have applied include Gibbs ensemble and semigrand ensemble MC, multi-histogram reweighting and the cumulant intersection method, whereas for the IE description of the phase diagrams we use the Ornstein-Zernike equation in combination with either the Duh-Henderson closure relation [3] or the soft mean spherical approximation (SMSA).
We present constant pressure and temperature sections of the phase diagrams for three selected Ising mixtures with different system parameters. The results show that on the one hand the simulations reproduce the mean field topology in the accessible temperature range, and on the other hand the IE calculations allow a quantitative comparison with the MC data.
Supported by the Austrian Fonds zur Förderung der wissenschaftlichen Forschung, project No. P15247.

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Phase transitions in 2D XY-model with biquadratic exchange interaction

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One of the most popular models in the theory of low-dimensional magnets is, so-called, XY-model. Using this model it is possible to describe, for example, the three-component systems with weak interfacial interaction. Except the traditional systems with the bilinear exchange interaction, there are magnetics, which properties are determined by the invariants of the higher orders in spin variables. Thereat, it is of interest to investigate the XY-model with the biquadratic exchange interaction. The Hamiltonian of an easy-plane ferromagnetic with the account of the biquadratic exchange interaction can be written as

$$\begin{aligned}\hat{H} &= -\frac{1}{2}\sum_{n,n'} J(n-n')\left[S_n^x S_{n'}^x + S_n^y S_{n'}^y + \Delta S_n^z S_{n'}^z\right] - \\ &- \frac{1}{2}\sum_{n,n'} K(n-n')\left[\frac{\Delta}{3}O_{2n}^0 O_{2n'}^0 + O_{2n}^2 O_{2n'}^2 + O_{2n}^{xy} O_{2n'}^{xy} + \right. \qquad (1)\\ &\left. + \Delta\left(O_{2n}^{xz} O_{2n'}^{xz} + O_{2n}^{yz} O_{2n'}^{yz}\right)\right] + \Delta\beta\sum_n \left(S_n^z\right)^2 + \hat{H}_{mel} + \hat{H}_{el},\end{aligned}$$

where $0 \le \Delta \le 1$; O_{2n}^t are the Stivens operators ($t = 0, 2, xy, xz, yz$); $\hat{H}_{mel}$ and $\hat{H}_{el}$ are the operators of magnetoelastic and elastic energies of the system. If the parameter $\Delta = 0$, then the Hamiltonian (1) describes the XY-model with the account of the biquadratic interaction. If $\Delta = 1$, then Eq. (1) corresponds to the three-component model. The account of the magnetoelastic interaction results in the stabilization of the long-range magnetic order in 2D-system.
Using the diagram techniques for the Hubbard operators, we determined the spectra of the magnetoelastic waves. The analysis of the spectra of elementary excitations allows us to plot the phase diagram of the system for an arbitrary Δ. Besides, we obtained the dependences of the points of the phase transitions on the material constants and the transition temperatures as the functions of the parameter Δ.

Magnetoelastic mechanism of the domain formation in antiferromagnets

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Existence of the domain structure (DS) in antiferromagnetic crystals (AFM) is experimentally ascertained and is beyond the question. Nevertheless, mechanism of this phenomenon is still unclear. In contrast to ferromagnets that posses macroscopic magnetization, AFM have no visible source of long-range forces of magnetic origin that may stabilize equilibrium inhomogeneous state.

In the present communication we argue that the internal mechanical stresses that accompany AFM ordering are the potential sources of long-range "destressing" fields. Due to magnetoelastic coupling, "orientations" of the internal stress tensor and AFM vector are tightly related. Spatial distribution of both values is defined by competition between the "easy" direction inside the sample governed by magnetic forces and preferable orientation of stress tensor at the sample surface.

In the finite-size samples the destressing fields result in either appearance of equilibrium DS that may be reversibly changed by application of external (magnetic, mechanical) field or a shape-induced anisotropy that may be detected by torque measurements.

Hall effect in organic layered conductors

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Galvanomagnetic phenomena in organic layered conductors with the quasi-two-dimensional electron energy spectrum of an arbitrary form have been studied theoretically.

We have obtained the asymptotic expression for the Hall field and magnetoresistance of a conductor placed in a strong magnetic field $\mathbf{H}$, when the cyclotron frequency Ω of electrons exceeds significantly their collision frequency $1/\tau$, for different orientations of $\mathbf{H}$ with respect to the layers.

It is shown that at low enough temperature, when the temperature smearing of the Fermi distribution function for charge carriers is much less than the separation between quantized Landau levels, in conductors with the Fermi surface consisting of topologically different elements, the amplitude of the quantum oscillations with $1/H$ of the Hall field is sufficiently large and comparable to the amplitude of the Shubnikov-de Haas magnetoresistance oscillations. In the case when the Fermi surface has the form of a single weakly corrugated cylinder in the collisionless limit ($\tau \to \infty$) the Hall field has no quantum corrections.

Experimental studies of the Hall effect along with the H-dependence of the magnetoresistance at different orientations of the magnetic field make it possible to determine in detail the topological structure of the Fermi surface, contribution into the electrical conductivity of different charge carriers groups and some other details of the electron energy spectrum of layered conductors.

Kinetic equations approach to the description of chemical reactions between adparticles at a metallic surface

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We carried out the investigation of reaction–diffusion processes at the metallic surfaces on the basis of the generalized Hubbard model with taking into account a substrate–adsorbate interaction by means of the method of quantum kinetic equations. Adparticles are supposed to be localized at the lattice sites; local equilibrium ionic potential forms the oscillatory states within each potential well. The model assumes site-to-site tunneling of the adsorbate, intrasite oscillation of the adparticle between the ground and excited states within a potential well, interaction of the adparticles with the lattice (coupling with the substrate is realized both by density and oscillation modes), and the occurrence of chemical reactions. The subject of interest is the system of kinetic equations of the reaction-diffusion type for a nonequilibrium one-particle distribution function of the adsorbate at the assumption of a phonon bath. The kinetic kernels describe cross-correlations of the different processes in the system and are studied both in low-temperature and in high-temperature regimes. The latter regime supposes adparticle self-trapping and suppression of the certain reaction channels.

Simulational studies of the random-site Ising model criticality

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We apply numerical simulations to study the criticality of the 3D Ising model with random site quenched dilution [1]. The emphasis is given to the issues not being discussed in detail before. In particular, we attempt a comparison of different Monte Carlo techniques, discussing regions of their applicability and advantages/disadvantages depending on the aim of a particular simulation set. Moreover, besides evaluation of the critical indices we estimate the universal ratio Γ^+/Γ^- for the magnetic susceptibility critical amplitudes [2]. Our estimate $\Gamma^+/\Gamma^- = 1.67 \pm 0.15$ is in a good agreement with the recent MC analysis of the random-bond Ising model [3] giving further support that both random-site and random-bond dilutions lead to the same universality class.

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Electrolyte distribution around two like charged rods and their effective attractive interaction

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We explored several conditions under which, two charged rods immersed in a primitive model electrolyte, experiment attraction. We found that attraction may occur even if the salt and counterions are monovalent at sufficiently high particles volume fraction. For divalent electrolytes, attraction occurs only if salt concentration is sufficiently high. These findings point out the relevance of considering properly the entropic contribution to the effective rod-rod interaction. We provide an analysis in which the effective interaction is discussed in terms of the electrolyte structure around the rods: there is a direct correlation between an angular charge reversal to attraction. Our results are computed by means of integral equations theories, the mean field Poisson-Boltzmann theory, and Monte Carlo simulations. Integral equations and computer simulations are in good agreement whereas Poisson-Boltzmann theory does not predict attraction.

Ion association in non-aqueous electrolyte solutions from a molecular modelling point of view

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A quantitative description of ion association phenomena in non-aqueous electrolyte solutions (NAES) especially with moderate and low dielectric constants remains a challenge for the contemporary condensed matter theory. To elucidate some questionable points concerning of ion association in the NAES a series of Molecular Dynamics (MD) and Brownian Dynamics (BD) simulations on several chosen NAES have been carried out. The role of different criteria of ion clusters definitions and calculated parameters of ion aggregation (lifetimes, constants of ion pairing, etc.) are discussed.

Nonequilibrium phase transitions in stochastic systems induced by noise cross-correlations

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A general approach for treating the spatially extended stochastic systems with the nonlinear damping and correlations between additive and multiplicative noises is developed. Within the modified cumulant expansion method, we derive an effective Fokker-Planck equation with stationary solutions that describe the character of the ordered state. We find that the fluctuation cross-correlations lead to a symmetry breaking of the distribution function even in the case of zero-dimensional system. In a general case, continuous, discontinuous and reentrant noise induced phase transitions take place. It appears that the cross-correlations play the role of bias field which can induce a chain of phase transitions of different nature. Within the mean field approach, we give an intuitive explanation of the system behavior by an effective potential of the thermodynamic type. This potential is written in the form of an expansion with coefficients defined by the temperature, intensity of spatial coupling, autocorrelation and cross-correlation times and intensities of both additive and multiplicative noises.

Above theoretical approach is mapped to the investigate the process of reconstructing the defect structure in the course of plastic flow. We introduce a phenomenological model which allows to take into account the transformation of mobile dislocations into the point defects and vice versa as well as the interaction between density of dislocations and macroscopic characteristics of deformation, spatial inhomogeneouity of the distribution of defects in crystal and the fluctuations of deformation and density of defects. Basing on a kinetic approach we show the correlation between fluctuations leads to the appearance of intermediate metastable phases which indicate the formation of clusters of dislocations with redirected Bürgers vector.

Thermoelectromechanical waves in superfluid helium

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In work [1] the polarization was experimentally registered in the absence of external electric field when thermally exciting the second sound wave in superfluid helium. The resonant excitation of second sound waves by oscillating electric field at that same frequency was carried out there for the first time. The amplitude of potential corresponding to polarization had the same resonant pattern as the thermal field at the frequency of the second sound wave. This testifies that the thermal and electric fields take part at the common oscillatory process and are connected with a linear relation. Such a link in the solid state physics exists in the piroelectrical effect. Actually this effect is what was observed in [1].

Having made a single assumption about adiabatical modulation of the energy of quasiparticles of He II (phonons, rotons), it is possible to find the appropriate additives to the equations of two-fluid hydrodynamics containing electrical fields, the induction caused by polarization and the expression for piroelectrical coefficient. The linearized equations of non-dissipative two-fluid hydrodynamics in this case describe the waves of first and second sounds, which are actually the thermoelectromechanical waves in this case. The possibility of existence of such kind of waves in piroelectrical crystals was studied in work [2]. The flat waves solution of these equations gives us the mutual links between the amplitudes of velocities of n- and s-components, pressure, temperature and electrical field in the first and second sounds. It appears that in the first sound wave the deviation of temperature and electric field are small comparatively with the deviation of pressure. In the second sound wave the link between the deviations of temperature and the electric field is more essential then between those quantities and the deviation of pressure. This explains the observation of the electric field during thermal excitation of second sound waves and its absence at the excitation of first sound waves.

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Synergetics of phase dynamics of ultrathin lubricant film

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Using the Lorenz model for viscoelastic medium approximation the melting of ultrathin lubricant film is studied by friction between atomically flat surfaces. The fluctuations of lubricant temperature are taken into account defined by Ornstein-Uhlenbeck process. The behaviour of the most probable shear stress, appearing in the lubricant, is studied and phase diagrams are calculated. The cases of second-order and first-order transitions corresponding to the melting of amorphous and crystalline lubricant are considered. It is shown that for the first case the fluctuations of lubricant temperature result in appearance of stick-slip friction domain, dividing the regions of dry and sliding friction, inherent in the first-order transition. In the second case the three stick-slip friction domains arise characterized by transitions between dry, metastable, and stable sliding friction. The increase of correlation time of lubricant temperature fluctuations leads to increasing of frictional surfaces temperature needed for realization of sliding friction.

The phase portraits are defined meeting the different regions of phase diagrams and determining system's kinetics. It is shown that the singular point, meeting the mode of dry friction, has indefinite character of stability, since phase trajectories exist converging to this point and diverging away from it. The other stable and unstable states of the system, corresponding to the extremums of distribution function, are presented by the center-type singular points on phase portraits. Consequently, the system can demonstrate oscillations near these points, thus they are set by concentric ellipses representing limit cycles. Presumably, such oscillations are caused by the presence of noise. The large extension of depicting

trajectories near centers along the axes of phase plane testifies to stability of sliding friction. In the last case, lubricant becomes more viscous and, vice versa, more fluid-like periodically, but it has a liquid-like structure in both cases. Since maximums of distribution function, separated by the expressed minimums of probability, correspond to the steady-state modes of friction, the transitions between them occur after large intervals of time.

Electronic structure of large modified nickel nanoclusters

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A combined method of semiempirical quantum chemical (MNDO) and classical molecular dynamics calculations was proposed and tested to study electronic and geometrical structures of large modified nickel nanoclusters. The cluster contained from 2 to 500 atoms of pure nickel atoms and to 100 atoms different kings (Pt, Pd, Cu, Mn, and Cr) in surface layer (111) with high symmetry. The following tendency showed stabilization of nanoclusters during complete geometry optimization with the growth of cluster sizes in all directions. A large cubooctaedral Ni_{485} was the most stable and had the lowest deflection from the real f.c.c. monocrystal in the metal volume. The cluster, constructed of 13 and 55 atoms in high symmetry, also presented relative stability by means of molecular mechanics and MNDO approach. Modified with noble metal (to 10%) cluster Ni_{485} was less stable (95% as compared with pure original nickel nanoclusters) and Ni–Cu cluster (10% Cu) had worse stability (73%). In contrast the clusters with Cr and Mn implanted atoms, presented nice stability. All cases were in vacuum, but in the environment of active gases, namely molecular oxygen, Ni–Pd and Ni–Pt nanoclusters kept on their stability, especially in the range of noble atoms, whereas Ni–Cu. Ni–Cr and Ni–Mn nanoclusters were actively oxidized and lost their surface stability.

All the examples may be useful in the search of stable large nanoclusters of transition metals, widely applied inheterogeneous catalysis with important practical applications (utilization of harmful gases and liquids, organically and inorganically synthesis.

Ferroelectric-antiferroelectric mixed systems. Equation of state, thermodynamic functions

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The quasi-spin model of ferroelectric-antiferroelectric mixed system[1] is discussed in details. The main peculiarity of the model are a possibilities for a site dipole momentum to be oriented ferroelectrically in the z-direction and antiferroelectrically in the perpendicular x-direction of a crystal. Such situation take place in hydrogen bonded mixed compounds of KDP type[2].

For taking into account the random distribution of z and x oriented dipole momentum we use the replica method[3,4]. As a result the partition function of the investigated system and it's free energy are obtained and analyzed.

The phase diagrams for the mixed system are investigated in details. It has been shown that ferroelectric and antiferroelectric phases exists only separately. But there is a possibility to observe mixed para-ferro, para-antiferro, dipole glass-ferro and dipole glass-antiferro phases also. The set of equation for ferroelectric, antiferroelectric and dipole glass order parameters is obtained. The dependence of order parameters on concentration and temperature are analysed. The behaviour of dielectric susceptibility in a wide temperature and concentration regions is founded.

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

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For description of thermodynamic and dielectric properties of the $Rb_{1-x}(NH_4)_xH_2PO_4$-type proton glasses, a pseudospin model with competing short-range and long-range interactions and random internal fields is proposed. Within a symmetric replica approach, a four-particle cluster approximation for the short-range interactions and a mean field approximation for the long-range interactions are used. Within the Glauber kinetic approach, a system of equations for a linear response of polarization and proton glass order parameter is derived. A qualitative description of the phase diagrams, thermodynamic and dielectric properties of $Rb_{1-x}(NH_4)_xH_2PO_4$ and $K_{1-x}(NH_4)_xH_2PO_4$ systems is obtained. Origin of a low-temperature peak in the imaginary part of the longitudinal permittivity in proton glasses is discussed.

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Calculation of electron-density profiles of semibounded metal, which is placed in external electric field

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Calculation of electron-density profiles of semibounded metal in jellium model is made by means of method functional integration. Advantage of this method is correct account of exchange and correlation effects wich is the problem in other approaches. The method which is presented allows to take into account an influence of electric field on the metal without recourse of the perturbation theory that allows to consider very strong electric fields. As illustrated in, that shift of metal electron density inside or outside of the metal depends on the direction of electron field which is applied.

Conformation of intertwining polymeric chains in the concentrated solutions and melts in the self-avoiding random walks statistics

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It was proposed a strict statistics of self-avoiding random walks in the d-measured lattice and continuous space for intertwining chains in the concentrated solutions and melts. On the basis of this statistics it was described the thermodynamics of conformation and isothermal and adiabatic deformation of intertwining chains. It has been obtained the equation of conformational state. It was shown, that in the field of chains overlap they are stretched increasing its conformational volume. In this volume there are others chains with the formation of m-ball. Free energy of a chain conformation does not depend upon the fact, if the chains intertwined or they are isolated in the m-ball. Mixing entropy is responsible to the chains interweaving in the m-ball. Dependencies of the conformational radius, free energy and conformation pressure on respective concentration of polymeric chains have been determined.

The liquid-vapour coexistence of simple fluids confined in disordered matrix: A new approach in the theory of associative fluids

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The knowledge of the properties of the sorbed fluids in specific porous solids is of great interest for both fundamental and applied sciences. Within the framework of the integral equations theory a porous medium involving the fluid is usually treated as a partly quenched system. The space between the quenched particles of the system as constituents of disordered matrix forms a random network of pores in which the molecules of adsorbed fluid are present. The most intriguing aspect of the study of the liquid-vapor phase behavior of a fluid confined in a matrix is related to the fact that some computer simulations give the evidence for two phase transitions: one is analogous to the liquid-vapor coexistence in a bulk fluid while the other still do not have such obvious interpretation. The results obtained within various theoretical approaches for the similar phase coexistence appear to be puzzling and very sensitive to the approximations applied. The problems are connected with the fluid critical temperature decreasing in the presence of a porous medium. It is known that at low temperatures the role of the attraction between fluid particles becomes very important. Therefore, association phenomena appear even in the case of a simple fluid and they can be treated by the statistical mechanics theory of associative fluids. We apply the method based on the replica Ornstein-Zernike equations within the associative mean-spherical approximation (AMSA) combined with the second coefficient of the optimized cluster expansion (OCE) in the limit of weak association. This approach allows us to estimate approximately the sum of the whole OCE for the free energy of the system in which two-particles association is most essential.

Using the approach proposed we calculate a series of phase diagrams of simple fluid confined in disordered matrix of various porosity. The attractive interaction leads to the change of the critical temperature. The effects of the strength of the fluid-matrix attraction on the critical parameters are discussed. The results obtained are compared with the computer simulation data as well.

Influence of the structural disorder on impurity states in liquid metal

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The given paper is devoted to studying of the impurity states of gaseous impurities O, F, C, Cl in melts of alkaline metals. Generalized model Hamiltonian includes the processes of elastic and non-elastic conduction electrons scattering on the charged impurity. Formation of a charging state of an impurity is interpreted as process of hybridization of conduction electrons on local degenerate s-level. Hybridizing terms of a Hamiltonian contain contributions from potential fields of a local environment of the impurity atom and depend on structure of the nearest order.

Using two-time temperature Green functions within Hartree-Fock approximation the system of a self-consistent equations for average thermodynamic occupation numbers of filling of the localized level is received. Charged and spin-polarized impurity states are evaluated corresponding to the quasi-crystalline case. Configurationally averaged one-particle Green functions are obtained, a short-range order of atomic configuration in a liquid metal is taken into account. The influence of structural disorder of a metal matrix on quantum impurity states which leads to an additional broadening of the localized level of an impurity is analyzed. It is mentioned that the present theory is applicable to liquid alkali metals with small concentration of gaseous impurities.

First-passage time: A conception leading to superstatistics

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To describe the nonequilibrium states of a system we introduce a new thermodynamic parameter - the lifetime (the first passage time) of a system. The statistical distributions that can be obtained out of the mesoscopic description characterizing the behaviour of a system by specifying the stochastic processes are written. Superstatistics, introduced as fluctuating quantities of intensive thermodynamical parameters, are obtained from statistical distribution with lifetime (random time to system degeneracy) as thermodynamical parameter (and also generalization of superstatistics). Necessary for this realization condition with expression for average lifetime of stationary statistical system obtained from stochastical storage model is consisting. The obtained distribution passes in Gibbs distribution depending on a measure of deviation from equilibrium related to fluxes and dissipativity in the system.

Energy spectrum of the organic quasi-1D conductor with NNN and correlated hopping

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In this work a model of organic quasi-one-dimensional conductors $(TMTTF)_2X$ and $(TMTSF)_2X$ is considered. The anisotropic character of these compounds is described by two different hopping parameters: t between nearest neighbors (NN) in a chain of tetramethyl-tetrathiafulvalene (TMTTF) molecules or tetramethyl-tetraselenfulvalene (TMTSF) molecues and t' between the chains (NNN - between next nearest neighbors). Similar models are studied intensively in connection with pseudogap phenomena in high temperature superconductors [1,2]. We also take into account correlated hopping of electrons and this allows us to describe the influence of site occupancy on hopping processes. The Coulomb repulsion between electrons is described by one-site (Hubbard) term.

In a regime of strong intra-atomic correlation we cut off high energy processes of doublon formation by applying two successive canonical transformation and obtain an effective Hamiltonian for the case of electron concentration $n < 1$. This Hamiltonian contains kinetic exchange terms of antiferromagnetic (AF) nature. Oppositely, NNN hopping and correlated hopping disfavor AF order, the latter, beside that, leads to spin-dependent subband shifts. The energy spectrum of the effective Hamiltonian is calculated by means of non-perturbative approach, namely projection procedure [3] for sequence of equation in Green function technique. With use of this spectrum sublattice magnetization can be calculated as a function of model parameters and temperature. Application of the obtained results to quasi-one-dimensional conductors is discussed.

This work was supported by Ukrainian Fund for Fundamental Research under grant No GP/F8/44

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Kinetics of a system in external random field with small correlation time. Higher order approximation

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Kinetics in the presence of a random field $\tilde{h}_i(t)$ has been studied on the base of a general equation for reduced description parameters $\eta_a(t)$ in a slow external field $h_i(t)$:

$$\partial_t \eta_a(t) = L_a(\eta(t), h(t)). \tag{1}$$

It is implied that $\tilde{h}_i(t)$ is a stationary Gauss process (random values are marked with a tilde) with short correlation time $\tau_0 \ll T$ ($\partial_t \eta_a(t) \sim \eta_a/T$). Equation (1) produces a random process $\tilde{\eta}_a(t) \equiv \eta_a(t, \eta_0, \tilde{h})$ ($\eta_a(t, \eta_0, h)$ is solution of the Cauchy problem for (1), $\eta_a(0, \eta_0, h) \equiv \eta_{a0}$), which is described by us with average values $\mathrm{f}_a(t)$ of $\tilde{\eta}_a(t)$ and their equal time correlations $g_{a_1 \ldots a_s}(t)$. The goal of the present work is to obtain a closed system of equations for $\mathrm{f}_a(t)$ and usual generating function for correlations $G(g(t), u)$ (u_a are auxiliary variables). The consideration is based on the Furutsu-Novikov formula and expansion of function

$$\nu_{ai}(t, t', \eta_0, h) \equiv \frac{\delta \eta_a(t, \eta_0, h)}{\delta h_i(t')}, \quad (\nu_{ai}(t, t', \eta_0, h) = 0, t' > t) \tag{2}$$

in the Tailor series at $t' = t - 0$. This reduces the considered problem to calculation of the following average values

$$\Phi_{a_1 \ldots a_s}(t, u) \equiv \overline{\tilde{h}_{a_1}(t) \ldots \tilde{h}_{a_s}(t) \exp \sum_a \tilde{\eta}_a(t) u_a} \tag{3}$$

in the terms of $\mathrm{f}_a(t)$ and $G(g(t), u)$. For the functions (3) a closed system of equations was obtained that is solvable in a perturbation theory in τ_0/T.

This work was supported by SFFR of Ukraine (project No. 2.7/418) and in part by INTAS (project No. 00-577).

Non-universal critical behavior of a mixed-spin Ising model on the generalized Kagomé lattice

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It is shown that the mixed spin-1/2 and spin-3/2 Ising model on the generalized Kagomé lattice is being equivalent to the eight-vertex model. Letting the parameter of uniaxial single-ion anisotropy $D \to \pm\infty$, the model becomes exactly soluble as a free-fermion eight-vertex model. Under this condition, the critical points are being characterized by critical exponents from the standard Ising universality class. On the other hand, in a certain subspace of interaction parameters corresponding to a coexistence surface between two ordered phases the model being exactly soluble as a symmetric zero-field eight-vertex model. This surface is bounded by a line of bicritical points that have remarkable interaction-dependent critical indices.

Critical parameters and pair correlations in confined multicomponent liquids

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In recent years in studying of critical phenomena and phase transitions significant results were obtained, especially for one-component and binary liquids, simple ferromagnets and so on. Nevertheless information about density (concentration) fluctuation correlations in multicomponemt systems, most of all confined, is limited. Here we consider pair correlations in liquid multicomponent finite-size system with geometry of a plane-parallel layer. For this system we find general expressions for pair correlation functions of density fluctuations. We also investigate influence of space limitation on correlative behavior of the system at critical region. The results are compared with those that exist for binary and pure liquids and their applicability is discussed briefly.

Statistical Physics 2005:

Modern Problems and New Applications

Posters

28–30 August 2005, Lviv, Ukraine

Critical indices calculations with small parameters

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The inequalities for the values of critical indices have been investigated in the work

$$\nu < 2/3, \qquad \xi > 2/5, \qquad \gamma < 4/3, \qquad \delta < 5, \qquad \beta > 1/3. \quad (1)$$

They follow from fluctuation theory of phase transition [1] and analyze of gravity effect data [2].

Small parameters $\gamma_0 = 4/3 - \gamma \ll \gamma$, $\delta_0 = 5 - \delta \ll \delta$ and so on were inserted on the basis of (1). It allowed to propose two new relations between the critical indices of the field and temperature dependences of correlation length and heat capacity in error at most $(1-2)10^{-3}$:

$$\nu^2 = \xi, \qquad \eta = \alpha_\mu/(1-\alpha_t). \quad (2)$$

These relations together with [1] gave to us possibility [2] to derive the equations, which determine the values of critical indices:

$$\nu^2 + 0.096\nu - 0.464 = 0, \qquad \xi^2 - 0.937\xi + 0.215 = 0 \quad (3)$$

($\xi = \nu^2 \approx (2/\pi)^2 = 0.405$). It is seen that the values of critical indices calculated on the basis of (3) are most close to the calculations of the 3-dimentional Ising model [1].

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Renormgroup approach for determine of magnitude of fluctuations interior field

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An inhomogeneous liquid was investigated near the critical point earlier [1] by using different experimental methods (refractometry, light and neutron scattering) and modeling on the basis of fluctuation theory of phase transition. It has been shown that in this case the internal field $|\Delta U(h)| = |\Delta\mu(h)| = |(\mu(h) - \mu_c)/\mu_c| \gg h$ is created under acting of gravitation field $h = \rho_c g \Delta_z P_c^{-1}$. The magnitude of the internal inhomogeneous field of fluctuations was investigated for inhomogeneous liquid under gravity near the critical point by the renormgroup approach. The chemical potential $\Delta\mu$ plays a role of field variable for the critical point. In fluctuation region (Wilson variant [2] of renormgroup) when nearing to the critical point the value, $\Delta\mu$, is renormalized in accordance to the renormgroup approach as follows:

$$\Delta\mu^* = \Delta\mu \cdot s^{1/2\cdot(3-\eta)+1)}, \qquad s \geq 1. \quad (1)$$

The renormalization arises after the consecutive Kadanov and scale transformations. It can be carried out until the size of subsystem does not reach the size of correlation length $r \sim R_c$ [3]. The collective behavior of molecules in correlated volume is determinative for the near-critical system. In this case it follows [2] from (1) and inequality $1/2\cdot(3-\eta)+1 > 0$ that the renormalization leads only to the increasing of the chemical potential $\Delta\mu^*$. The field variable of hydrostatic pressure h is an external variable and it's not renormalized. It follows from here that $\mathrm{d}\mu^*/\mathrm{d}h > 1$. This conclusion for inhomogeneous system near the critical point is approved by all existing experimental data on gravitational effect.

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Study of magnesium oxide properties in polarization model

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In recent years magnesium oxide has become the subject of increasing theoretical interest. Its properties have been studied using both ab initio Hartree-Fock technique and molecular models. These approaches, however, come across with certain difficulties. Ab initio methods allow to study crystalline properties from the atomic scale, but they are applicable to relatively small systems only. It is not possible to describe both bulk and diatomic molecule properties of magnesium oxide with the same set of interionic potentials, because of highly ionic character of its crystal bonding and a significant covalent contribution to the molecule binding energy.

We present a polarization model which allows to take into account coordination number and enables us to determine surface potential of bounded crystals with simulation methods. Switch out function was used to represent proton screening on phenomenological level, i.e. the covalency of the bonding to some extent. On the basis of ab initio calculation data on interaction potential curves Mg...Mg, O...O, Mg...O short-range contributions were obtained. Spline interpolation was used in further calculations involving these potentials. Surface properties of different-size magnesium oxide clusters were studied in the frames of proposed model. It was shown that collective effects make a significant influence on the ion state in the clusters. Comparison of cluster characteristics with ab initio calculations shows good coincidence of results. Proposed approach can be applied to a wide variety of materials.

Soliton-like order parameter distributions in the critical region

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Some exact one-component order parameter distributions for the Michelson thermodynamic potential are obtained. The exact partial distribution with energy, which is lower at some temperature interval than for the best of the known order parameter models in the form of the elliptic Jacobi functions, is obtained for the thermodynamic potential of the Ginzburg-Landau type.

Application of the collective variable method in the statistical thermodynamics of ion system in porous medium

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Thermodynamic characteristics of an ion system in a porous medium are calculated. The calculations are made within the classical collective variables method. The cases of both ion and non-polar dielectric porous matrices are considered. The calculations are made in the random phase approximation (RPA) as well as with the first virial coefficient taken into consideration. The expressions for the free energy, mean energy, and the equation of state are obtained. It is shown that in RPA these formulae differ from the respective relations for "non-quenched" particles by a certain factor (less than unity) being dependent on the porosity and not dependent on the volume and temperature. That is, porosity stipulates only the quantitative changes (namely, decreasing) of the thermodynamic functions. However, when the first virial coefficient is taken into account, the mentioned factor is already dependent on the volume and temperature. This fact leads to the qualitative changes of the thermodynamic characteristics.

The calculations are made using both the replica method and the direct averaging of the free energy of ion sub-system over the Gibbs distribution of the porous medium.

Behavior of passive admixture in vortex hydrodynamic field

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Passive admixture of spherical particles in the stationary hydrodynamic field of vortex drain positions at equilibrium circle orbit, at which the centrifugal force is compensated by radial force of hydrodynamic resistance. It is shown that with the existence of attraction and repulsion forces between admixture particles, the cluster structures of particles appear in the cortex stream and each accumulation turns in a circle at selected orbits. This leads to the separation between liquid and admixture. If particles are initially placed in the nodes of equilateral triangles, then after some time six independent cluster structures appear. Results are studied using the molecular hydrodynamics methods in the heterogeneous hydrodynamic field for the hundred of particles with pair interaction potential (modified Morse potential).

The theory of Brownian motion of weak solution of admixture in heterogeneous stream near the equilibrium orbit with the suitable edge conditions is built. The analysis of single-particle distribution function and its moments depending on the parameters of hydrodynamic flow is conducted.

The hydration structure of hydrophobic chain-like molecules with side hydrophilic groups: An ab initio molecular dynamics study

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The aim of this study was to explore by the ab initio molecular dynamics approach changes in the geometry of chain-like molecules, which contain hydrophobic and side hydrophilic groups, during the hydration process. We have performed an electron density functional study of equilibrium geometry of molecules CH_3–CH_2–CHOH–CH_2–CH_3 and CH_3–$[CH_2$–CHOH$]_2$–CH_2–CH_3. The calculations on the second type of molecule were needed in order to understand the tendency in geometry of the chain-like molecule with increasing number of [CH_2–CHOH] groups. All the calculations were performed in frames of ab initio density functional approach with the Vanderbilt type of pseudopotentials, and the gradient corrected functional in Perdew-Burke-Ernzerhof formulation. The interatomic distances and molecular angles for the molecule CH_3–$[CH_2$–CHOH$]_2$–CH_2–CH_3 were obtained in good agreement with Jorgensen's parameters used for organic molecules. The geometry minimization procedure for hydrated by thirty two water molecules CH_3–$[CH_2$–CHOH$]_2$–CH_2–CH_3 at the temperature 293 K was performed within the framework of electronic density functional approach. Optimization of hydration structure permitted both redistribution of electronic density in molecules CH_3–$[CH_2$–CHOH$]_2$–CH_2–CH_3 and H_2O, and displacements of ions towards local energy minima. As a result of hydration the geometry of the molecule CH_3–$[CH_2$–CHOH$]_2$–CH_2–CH_3 was changed. In contrast to non-hydrated molecule both OH groups of the molecule CH_3–$[CH_2$–CHOH$]_2$–CH_2–CH_3 are not parallel anymore, there exists an angle of approximately 60 deg between them. Hence, our calculations of hydration structure of the molecule CH_3–$[CH_2$–CHOH$]_2$–CH_2–CH_3 by the ab initio molecular dynamics point out on the probable changes in orientation of the hydrophilic groups OH due to interaction with the water molecules.

Coexisting of magnetic ordering and superconductivity in a iodine doped Bi2234 high temperature superconductors

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We research the phase interaction and phase transformation in $Bi_{1.6}Pb_{0.4}Sr_2Ca_3Cu_4O_{12-Y}$ – BiOI system and modification of superconducting and magnetic properties of these compounds by method of the "anion(oxygen) - anion(iodine)" substitution. The synthesis of the 2234 phase take place in the narrow temperature interval 840°–850° C in presents of Pb ions, BiOI powder and with Ca/Sr > 1.

Introduction of halogen into $Bi_{1.6}Pb_{0.4}Sr_2Ca_3Cu_4O_{12-Y}$ results in a change of melting character into quasicongruent one. Significant increasing in microhardness of samples and decreasing in their porosity, which was observed, has the positive influence on superconductive parameters of these compounds.

We observed two superconducting transitions in the temperature region 60–110 K with $T_{c1} = 108$ K ("high-T_c" phase) and $T_{c2} = 65$ K ("low-T_c" phase) for $Bi_{1.6}Pb_{0.4}Sr_2Ca_3Cu_4O_{12-z}I_z$ samples with $z > 0.025$, respectively. In the external magnetic field with magnitude higher as 2.5 T two magnetic phase transitions are observed: the first short-range antiferromagnetic ordering with $T_N = 67.8$ K and $\Theta_p = -31$ K; and second long-range ferromagnetic (or metamagnetic) ordering with $T_c = 14.625$ K and $\Theta_p = 1.5$ K.

The existence of competing ferromagnetic and antiferromagnetic interaction is not very surprising, because there exist no direct Cu-O-Cu superexange path in the $Bi_{1.6}Pb_{0.4}Sr_2Ca_3Cu_4O_{12-z}I_z$ structure, respectively: 1) $Cu^{2+}(d_{x^2-y^2})$–$O^{2-}(2p_y)$–$I^{1-}(3p_y)$–$Cu^{2+}(d_{x^2-y^2})$ - for the antiferromagnetic interaction, and 2) $Cu^{2+}(d_{z^2})$–$O^{2-}(2p_z)$–$I^{1-}(3p_z)$–$Cu^{2+}(d_{z^2})$ - for the ferromagnetic interaction. The mechanisms of appearing and coexisting of the magnetic ordering and superconductivity in these compounds are determined.

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Influence of an uniaxial crystal-field anisotropy on thermodynamic properties of the super-exchange antiferromagnetic Ising model

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Fisher super-exchange antiferromagnetic model on a square lattice is generalized by adding the uniaxial crystal-field anisotropy parameter on decorated atoms with an arbitrary spin S. The considered model in which the antiferromagnetic arrangment of spin-S atoms is realized via intermediate nonmagnetic atom, is exactly investigated within the framework of the generalized decoration-iteration mapping technique. An exact relation between partition function of the studied system and that one of the standard zero-field spin-1/2 Ising model on the square lattice is obtained. Exact results for the magnetization, specific heat, susceptibility, Gibbs free energy and enthalpy are obtained for arbitrary spin values S of decorated atoms. In particular, the simultaneous effects of the crystal-field anisotropy and external longitudinal magnetic field on thermodynamic properties is studied. The most interesting numerical results for the finite-temperature phase diagrams, thermal dependencies of the sublattice magnetization and other thermodynamic quantities are discussed in detail for the spin case S = 3/2.

The consistent description of kinetics and hydrodynamics of dusty plasmas in the self-electromagnetic field. Time correlation functions.

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Theoretical studies of non-equilibrium kinetic and hydrodynamic processes in dusty plasma remain actual in modern plasma physics. Dusty plasma differs from ordinary multicomponent plasmas that charges of grains are not fixed and depend on local conditions and plasma flows which charge a dust. Because the dust absorbs plasma particles, dusty plasma always is the open system, for which the source of ionization is necessary. The openness of such system can support self-organization processes in it. The problems of a description of processes in dusty plasma were considered in many works [1-3].

In our work, using Zubarev non-equilibrium statistical operator method a statistical description of dusty plasma in the self-electromagnetic field is performed. The generalized hydrodynamic transfer equations are obtained in which the transfer kernels renormalized taking into account kinetics of dust particles and depend on the state of electromagnetic field. In weakly non-equilibrium case the system of transfer equations for time correlation functions is derived and analyzed.

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Dynamics of dimer and z spin component fluctuations in spin-1/2 XX chains

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We consider the spin-1/2 XX chain in a transverse ($\parallel z$) magnetic field with the Hamiltonian

$$H = \sum_n J\left(s_n^x s_{n+1}^x + s_n^y s_{n+1}^y\right) + \sum_n \Omega s_n^z \qquad (1)$$

and examine the dynamic susceptibilities

$$\chi_{AB}(\kappa,\omega) = \sum_n \mathrm{e}^{\mathrm{i}\kappa n} \int_0^\infty \mathrm{d}t \mathrm{e}^{\mathrm{i}(\omega+\mathrm{i}\epsilon)t} \frac{1}{\mathrm{i}} \langle [A_j(t), B_{j+n}] \rangle\,, \qquad \epsilon \to +0 \qquad (2)$$

for the transverse spin component operator s_n^z and the dimer operator $D_n = s_n^x s_{n+1}^x + s_n^y s_{n+1}^y$ (see, e.g., [1]). Within the Jordan-Wigner fermionization approach these quantities are governed exclusively by the two-fermion excitation continuum. We discuss the meaning of our findings from the point of view of the linear response theory.

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Magnetic field dependence of conductivity and effective mass of carriers in a model of Mott-Hubbard material

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The influence of external magnetic field h on a static conductivity of Mott-Hubbard material which is described by model with correlated hopping of electrons has been investigated. By means of canonical transformation the effective Hamiltonian which takes into account strong intra-site Coulomb repulsion and correlated hopping is obtained. Using a variant of generalized Hartree-Fock approximation the single-electron Green function and quasiparticle energy spectrum of the model have been calculated. The static conductivity σ has been calculated by method of work [1] as a function of h, electron concentration n and temperature T. In the magnetic field σ reflects the changes of single electron energy spectrum through correlation narrowing of the band and shift of subband center. The temperature and concentration dependencies of σ are governed by changes of system magnetization in external magnetic field. We have found that in the ground state the saturated ferromagnetic state is stable while at non-zero temperature magnetization has the concentration dependence which agrees with work [2]. Such behavior of magnetization leads to $\sigma(n)$ dependence with maxima at quarter and three-quarter fillings in distinction from paramagnetic ones, obtained in work [1]. At non-zero temperatures the sharp changes of $\sigma(n)$ dependence are possible. It is due to complicated character of temperature dependence of band narrowing factor. Effective mass of quasi-particles appear to be spin-dependent and substantially varies with magnetic field. Taking into account the correlated hopping which is inherent to real narrow band materials allows us to interpret the peculiarities of conducting transition metal compounds.

This work was supported by Ukrainian Fund for Fundamental Research under grant No. 02.07/266.

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Magnetizations and critical temperature of amorphous binary alloy

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In this paper the generalized spin-electron model is used for description of magnetic states of amorphous substitutional alloys with the structural disorder of liquid type. Thermodynamical properties of $s-d$ model are investigated in the framework of the concept of order parameters. A scheme of consistent taking into account of the contributions of structural fluctuations (correlational spin-electron interactions and also the effects caused by scattering of conductivity electrons on structure fluctuations) to the thermodynamic functions and observable quantities is considered. Using the perturbation theory the functional of the thermodynamic potential is constructed as a functional power series.

From the self-consistency conditions of a minimum of thermodynamical potential with respect to the order parameters and the definition of polarization and the equation for the chemical potential of the electron subsystem of the alloy the equations for magnetizations and critical temperature of the paramagnetic-ferromagnetic transition are obtained. In work the figures of dependence of magnetizations from temperature and other parameters of model and also figures of temperature Curie are presented and analysed.

Exact ground-state diagrams for the generalized Blume-Emery-Griffiths model

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A simple way for constructing exact ground-state diagrams of classical spin models with nearest or (in certain cases) also with next-to-nearest-neighbor interactions is proposed for a large class of lattices. Such diagrams are constructed for the most general spin-1 Ising model on the unfrustrated lattices with nearest neighbor interaction. Nine topologically different diagrams are found. The same model is considered on the triangular lattice and on the square lattice with nearest and next-to-nearest-neighbor interactions. Intermediate nonuniform phases are revealed and the conditions of their nonexistence are obtained.

Study of the latex film formation process by Monte Carlo simulation

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Latex polymers have been widely employed in paints, adhesives, paper coatings, etc. Its exploit will increase beyond these current uses because they represent environmental friendly materials as they utilize water instead of organic solvents. One of the most important uses of dispersed polymers is in the form of organic coatings. Once the dispersion is over a substrate, water evaporates and it is possible to obtain a continuous polymer film. Polymer film properties as mechanical strength, opacity, permeability, among others, are affected not only by the nature of polymers but also by the film preparation conditions [1].

A simple model to study the latex film formation [2] was employed to study the influence of the solvent draying rate and polydispersity. Permeability properties of model latex film and film surface roughness were studied by computer simulation to characterize the formed films. It was shown how the high quality films over a flat substrate can be obtained at low drying rates and monodisperse polymer particles.

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On the critical dynamics of random anisotropy systems

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We study the purely relaxational critical dynamics with non-conserved order parameter (model A critical dynamics) for systems with disorder in form of random anisotropy axis. For the random axis anisotropic distribution, the static asymptotic critical behaviour coincides with that of random Ising systems [1]. Therefore the asymptotic critical dynamics is governed by the dynamical exponent of the random Ising model. However, the disorder influences considerably the dynamical behaviour in the non-asymptotic regime. We perform a field-theoretical renormalization group analysis within the minimal subtraction scheme in two-loop approximation to investigate asymptotic and effective critical dynamics of random anisotropy systems. The results demonstrate the non-monotonic behavior of the dynamical effective critical exponent $z_{\rm eff}$.

Acknowlegments for support of Fonds zur Förderung der wissenschaftlichen Forschung under Project No. P16574

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Non-dissipative drag in a two-component superfluid Bose gas: The microscopic theory

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For the first time the non-dissipative drag in multicomponent superfluids was described phenomenologically by Andreev and Bashkin with reference to ^{3}He–^{4}He mixtures. Later this idea was applied to bilayer superconductors and neutron-proton mixtures in neutron stars.

The experimental discovery of the Bose-Einstein condensation in alkali metal vapors and further progress in creating and manipulating of Bose-Einstein condensates (two-component, as well) allows to consider such systems as perspective objects for the observation of the non-dissipative drag effect.

In this report we present a microscopic theory of a non-dissipative drag in a two-component superfluid Bose gas. The theory is based on the formalism of the density and phase operators. The most general case of the system of two species of different densities, different masses and different interaction parameters is considered. The analytical expression for the drag current is obtained. It is shown that the drag current is proportional to the square root of the gas parameter. It is found that drag effect is maximal at zero temperatures. At non-zero temperatures the effect decreases but it remains of the same order as at $T = 0$, if temperature is comparable to the interaction energy.

The application of the theory to the alkali metal gases is discussed. A possible way of measuring the drag factor in a toroidal system with two Josephson barriers is proposed. It is shown that the measurement of the difference of number of atoms in two wells under a controlled evolution of the state of the system allows to determine the drag factor.

Kinetic equations for Bose systems with consideration of the large-scale hydrodynamic processes

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Investigation of the dynamic properties of quantum liquids, the features of transition from the vapor state into the liquid and superfluid ones under decreasing temperature is a topical problem of the modern condensed matter physics. One of the arising problems is to construct the nonequilibrium statistical theory, which would take consistently into account one-particle and collective processes, occurring in the system. Thus, there is an important problem of going out from the hydrodynamic region to the domain of intermediate values of wave vector and frequency, where the kinetic and hydrodynamic processes are interdependent and have to be considered simultaneously.

Using the method of nonequilibrium statistical operator, we proposed a new approach to the description of Bose system kinetics, with taking into consideration slow hydrodynamic transport processes. In such an approach, a nonequilibrium statistical operator has been constructed, that describes consistently both kinetic and nonlinear hydrodynamic fluctuations in a quantum liquid. Using this operator, we obtained the system of equations for one-particle Wigner's distribution function and for the functional of hydrodynamic variables (the densities of particle number, momentum and energy). Neglecting the hydrodynamical fluctuations, we obtain a traditional model of the kinetic theory.

CO oxidation on thin Pt crystals: stoichiometric and mathematical models taking into account the temperature balance

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We performed a stoichiometric analysis some of oscillatory chemical reactions in order to simplify the analysis of the process. Having considered the temperature balance equation, after equalization of elementary stages of the process and after introduction of corresponding changes into the stoichiometric matrix according to the principles of formal kinetics we obtained the final model for quantitative investigation of time characteristics of complex heterogenic processes in kinetic part. Comparison of quantitative results of model investigation with experimental data indicates that this model can be justifiably applied for processes in kinetic part of experiments.

Lys Mykyta and Zipf law

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The law observed by G.K. Zipf originally [1], describes the scaling dependence between the rank of the word k and frequency of its appearance

$$P(k) \sim k^{-\alpha}. \qquad (1)$$

Since its first observation in quantitative linguistics, the power-law dependence (1) was observed in numerous exotic problems of statistical physics, ranging from cell metabolism to sociophysics, econophysics, creation of musical context, etc. [2] and currently serves as an archetype of a scaling behaviour in complex systems.

The analysis of Zipf [1] was based on a large corpora of English, Latin, and Chinese texts. In our study, we analyze Ukrainian texts taking two masterpieces "Lys Mykyta" and "Abu-Kasym's shoes" by Ivan Franko as examples. Although our statistics involves rather short texts, nevertheless clear appearance of the Zipf law (1) with an exponent $\alpha \sim 0.98$ is observed. Moreover, we check whether the Simon's scenario [3] proposed to explain appearance of the Zipf law (1) holds for the text generation.

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Elastic properties of compressed rare-gas crystals

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An analytical expression for the energy (adiabatic potential) of a crystal was derived using Hartree-Fock method for rare-gas crystals (RGC). The short-range interaction, which is the most important part of the potential in case of high pressure was calculated from the first principles without any parameters. It allows one to utilise it for analytical calculations of phonon spectrums and elastic properties of insulators over a wide in range of pressure, up to the pressure of "insulator – metal" phase transition.

For the entire series of compressed RGC, we derived and solved the equations of states $p = p(V)$ and calculated the Brugger (C_{11}, C_{12}, C_{44}), Fuchs (B_{11}, B_{12}, B_{44}), and Birch $(\mathcal{B}_{11}, \mathcal{B}_{12}, \mathcal{B}_{44})$ elastic moduli in the nearest and next-to-nearest neighbour approximation using our interatomic potential. It is of interest to compare the behaviour of the shear modulus B_{33} as a function of the pressure for RGC. In particular, the elastic moduli B_{33} for Xe decrease as the compression increases and become zero when the compression $\Delta V/V_0$ reaches 0.7. This suggest that, under pressure, the Xe crystal should undergo a phase transition. In actual fact, a pressure-induced phase transition in solid Xe was experimentally observed. This is a transition from an intermediate close-packed phase to a hexagonal close-packed phase at $p = 0.75$ Mbar immediately prior to metallization observed under compression $\Delta V/V_0 = 0.7$ (1.5 Mbar).

The results of calculations $\mathcal{B}_{ik}$ are in satisfactory agreement with the experimental data. The dependence's $\mathcal{B}_{ik}$ remain linear at to 10 Mbar. The validity of Cauchy relation is confirmed in the most precise experiment for Kr. So the interatomic interaction in RGC has a central character. Thus, the comparison of the theory and experiment enables us to assert that the interatomic potential proposed accounts for all the important features in the behaviour of RGC under pressure.

Photo-induced deformations in azobenzene-containing side-chain polymers: molecular dynamics study

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Azobenzene-containing polymers are of considerable technological interest both as an optical storage media and in optical-only manufacturing of diffractive elements. A vast amount of experimental data have been collected on both optically induced surface relief grating formation or reversible contraction/extension depending on polymer architecture. However, the satisfactory theoretical explanation is still on its way.

We perform molecular dynamics simulation of model side-chain polymer system with azobenzene moietes. The effect of trans-cis-trans photoisomerisation is considered statistically, in terms of external reorientating optical field. The simulations are performed in constant-stress NPT ensemble allowing anisotropic changes of box dimensions.

As a result, the contraction of side-chain polymeric system in nematic and smectic phases is observed when illuminated by linearly polarised light (the effect observed in experiments on azobenzene-containing elastomers by Finkelman et al). The driving force is a photoinduced melting of nematic/smectic phase and repacking of azobenzenes, the effect similar to the raise of the temperature. To compress the time-scale of the simulations relatively strong external fields are used and the dependence of the effect on field strength is studied. We also perform conformational analysis of main and side chains during the illumination.

The simulations show the relevance of reorientational effects in photoactive behaviour of azo-polymers and are considered as a first step for more realistic modelling.

Thermodynamics and proton transfer in chain-like hydrogen bonded systems

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The studying of different classes of hydrogen bonded systems with strong correlations between protons on the neighboring bonds are presented. Starting from the concept implying the existence of the double well potential for the proton on each bond the original approaches are used for various systems with hydrogen bonds. The developed model with reduced basis is applied for H-bonded chains of finite length. In this model the proton states corresponding to the high-energy proton configurations are excluded from the initial basis in this model. It is shown that the such linear complexes can possess the special dependencies of thermodynamic functions on the number of hydrogen bonds N (polarizability $\sim N^2$ and specific heat $\sim 1/N$).

For linear H-bonded systems also is considered orientational-tunnelling model for description of proton transfer. The translation motions of protons in the double well potential within hydrogen bond as well as orientational jumps between neighboring bonds are taken into account. It is shown that the thermodynamic functions depend strongly on external electric field strength and on frequency of orientational rotations.

The processes of formation of hydrocomplexes in chain-like H-bonded structures with transuranium elements is considered.

Mathematical modeling and optimization of metabolic process in biotechnology

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From the point of view of industrial biotechnology metabolism is a formation of valuable biochemical products – some of them are exuded into the medium (extracellular products) and some are accumulated in biomass (intracellular products) – during the growth of microorganisms. Antibiotics, enzymes, polysaccharides and many other products are obtained during metabolism. The industrial production is directed on obtaining the highest outputs. Therefore, it is necessary to carry out an optimization of such technological parameters like:

– The yield of product in calculation on the consumed substrate;
– The content of nutrient medium and the regime of nutrition;
– The optimal values of temperature, pH, aeration.

Our system consists of multi-component input and output parameters. It is sufficiently difficult to investigate it by experimental approach only. In this case mathematical modeling of metabolic processes is necessary for finding the optimal conditions of conducting the process (regime of nutrition and fermentation) for the optimal synthesis of the necessary metabolites. For the modeling of synthesis processes we used self-organizing maps (SOM) and group method of data handling (GMDH) algorithms. Using SOM techniques we obtain SOM-maps that establish a new relationship in experimental data structure. Analysis of the obtained clusters was made by GMDH. As a result, mathematical modeling makes it much easier to investigate complex biochemical systems using modern computer tools to perform computer simulation. The new complex biotechnological product – biosurfactant, which is synthesized by the strain PS, has good perspectives of utilization in priority ecologically safe technologies. It is shown, that the properties of the product, the content and correlation of rhamnolipids, polysaccharides, enzymes, polypeptides etc. can be directly regulated with methods of mathematical modeling.

The work was carried out within the frame of GrantSTCU 3200.

Stochastic theory of self-similar mode of stick-slip boundary friction

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Using the Lorenz model the melting of ultrathin lubricant film by friction between atomically flat surfaces is studied. The additive noises of the elastic shear stress and strain, and the temperature in the film are introduced for building the phase diagram where the noise intensity of this temperature and temperature of friction surfaces define the domains of sliding, dry, and stick-slip friction. The conditions are found at which the last regime corresponds to the intermittency mode inherent in self-organized criticality phenomenon. The self-similar distribution of the stress is represented allowing for their nonlinear relaxation and fractional feedbacks in the Lorenz system and it is provided with temperature fluctuations. Such fractional scheme is used for building the phase diagram determining various modes of friction. The study of corresponding fractional Fokker–Planck equation shows that stick-slip friction corresponds to the subdiffusion process.

The self-similar behaviour of lubricant film is studied taking into account correlation fluctuations of its temperature defined by Ornstein-Uhlenbeck process. The behaviour of the most probable shear stress, appearing in the lubricant, is considered and phase diagrams are calculated. It is shown that the fluctuations of lubricant temperature result in disappearance of sliding friction region at presence of dry and stick-slip friction domains in both above cases. In the second case the stick-slip motion arises characterized by three stationary values of shear stresses at which dry, metastable, and stable sliding friction are realized.

The phase portraits are defined meeting the different regions of phase diagrams and determining system's kinetics. It is shown that the singular point, meeting the mode of dry friction, has indefinite character of stability, since phase trajectories exist converging to this point and diverging away from it. The other stable and unstable states of the system, corresponding to the extremums of distribution function, are presented by the center-type singular points on phase portraits. Consequently, the system can demonstrate oscillations near these points, thus they are set by concentric ellipses representing limit cycles. Presumably, such oscillations are caused by the presence of noise.

Thermomagnetic phenomena in layered conductors

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We have studied theoretically thermomagnetic and thermoelectric effects in layered conductors with a quasi-two-dimensional electron energy spectrum of arbitrary form in a quantizing magnetic field **H** at low temperatures.

Giant quantum oscillation of the thermoelectric field versus $1/H$, have been predicted, which will facilitates the experimental study of quantum oscillatory effects. The linear response of the electron system in a layered conductor to an external action in the form of an electric field and a temperature gradient is determined from the solution of the quantum kinetic equation for the statistical operator. The quantum oscillations of the amplitude of charge carriers scattering by impurity atoms have been calculated in the Born approximation.

Thermomagnetic coefficients of a layered conductor are shown to depend periodically upon the angle θ between the magnetic field direction and the normal to the layers. This orientation effect arises from the quasi-two-dimensional character of the charge carriers energy spectrum and is representative of layered conductors. We have obtained the oscillatory dependence on θ of both the smoothly varying part of the thermoelectric field and the amplitude of its quantum oscillations in the case when the temperature gradient is oriented along the normal to the layers. Analysis of this dependence makes possible to estimate the overlapping of wave functions for electrons belonging to different layers.

It is shown that joint experimental studies of galvanomagnetic and thermomagnetic effects will enable the quasi-two-dimensional electron energy spectrum in layered conductors to be determined in detail.

On statistical theory of nonequilibrium processes in nonuniform electron system of a metal surface

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Theoretical investigation of nonequilibrium processes in nonuniform electron system of the metal surfaces is a topical problem both from experimental (scanning tunnelling microscopy, field ionic microscopy and their modification) and theoretical point of view (more profound understanding of the mechanisms of diffusion, adsorption, desorption, catalytic reactions in various surface phenomena). In this report we present a statistical theory of nonequilibrium processes in nonuniform electron system of the metal surfaces in the framework of the method of nonequilibrium statistical operator. For the model of semi-bounded system "point ions — collective electrons" with chosen reference system of the "jelly" model we obtain a generalized quantum equation of electro-diffusion for the mean value of electron density operator. By the means of functional integration it has been calculated a statistical weight of quasiequilibrium statistical operator as a function of electrochemical potential of the electron system that depends on space and time variables.

Behaviour of the order parameter of the simple magnet in an external field

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Critical behaviour of an Ising-like system on the simple cubic lattice is studied in the collective variables (CV) method[1]. Within the framework of this method, we perform the integration of partition function over all CV ρ_k. The last step of calculation is the integration over the variable ρ_0 by the steepest descent method[2]. The free energy of the system contains the free energy of ordering determined by integration with respect to CV ρ_0, whose average value is proportional to the order parameter. This is the main contribution to the average spin moment of the system. The equation for this quantity is obtained and solutions as functions of the field and temperature are investigated. They contain the dependences on the microscopic parameters, in particular, on the lattice constant and interaction potential parameters. The physical solution corresponds to the free-energy minimum condition. The results of the calculation are demonstrated for the low-temperature region.

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On the theory of electrical conductivity in ionic liquids

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About 50 years ago from the analysis of experimental data a phenomenological 'universal golden rule' for the ratio of partial conductivities of ions in molten salts has been proposed [1]. This rule is expressed in very simple form $\sigma_+/\sigma_- = m_-/m_+$. Recently there were several theoretical attempts [2] to derive this relation using the equations of motion, the Langevin equation as well as molecular dynamics studies for the model of charge symmetrical molten salts.

In this report, starting from the rigorous relations derived us previously for the generalized transport coefficients of a multicomponent fluid [3], we consider this problem in more detail. In particular, it is shown that the 'universal golden rule' gives just one example of more general class of exact relations. For charge asymmetric model more general expression for the ratio (k, ω)-dependent partial conductivities is obtained

$$\frac{\sigma_+(k,\omega)}{\sigma_-(k,\omega)} = -\frac{q_+}{q_-}\frac{m_-}{m_+},$$

where q_α is a charge of ions in the αth species, $\alpha = 1, 2$.

This work is partly supported by the Fundamental Research State Fund of the Ministry of Education and Science of Ukraine under Project No. 02.07/00303.

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Theoretical investigation of the influence of tunneling effects upon physical characteristics of the Rochelle salt, RbHSO4 and NH4HSO4 crystals within the Mitsui model.

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We investigated the phase transitions in Rochelle salt, $RbHSO_4$, NH_4HSO_4 crystals within the mean field approximation for the Mitsui model taking into account tunneling effects. On the phase diagrams obtained for this model in work [1] the regions with the sequences of phase transitions occurring in Rochelle salt, $RbHSO_4$ and NH_4HSO_4 crystals were determined. We studied the possibility to find in these regions the points corresponding to the sets of model parameters, which could provide a satisfactory agreement between theoretically calculated thermodynamical properties of studied crystals and experimental ones.

For Rochelle salt, in particular, all calculations were made on the basis of Mitsui model taking into account tunneling effects and effects related to piezoelectric shear strain, spontaneous in the ferroelectric phase [2]. All thermodynamic, dielectric, elastic, and piezoelectric properties of Rochelle salt were calculated within this model and were compared to the experimental data. Investigating the influence of tunneling upon physical characteristics of Rochelle salt we revealed that considering tunneling improves agreement between a theory and experiment for polarization without affecting the agreement between a theory and experiment for other thermodynamic characteristics.

For $RbHSO_4$ crystal we discovered that taking into account the tunneling allows us to derive new sets of model parameters providing the same agreement between theoretically calculated thermodynamical properties and experimental ones as set of model parameters without tunneling. In general agreement between theoretically calculated and experimental physical properties was obtained quite satisfactory.

For NH_4HSO_4 crystal the agreement between theory and experiment within the model without taking into account tunneling effects can not be achived. Taking into account the tunneling effects allows us to derive the agreement between theoretically calculated and experimental physical properties except for the heat cappacity. It may be related to the error for experiment for this characteristic or with the error for the structure NH_4HSO_4 crystal.

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Thermodynamic characteristics of spin-1 Ising model with bilinear and quadrupolar interactions under magnetic field. Two-particle cluster approximation

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Influence of external magnetic field on spin-1 Ising model with bilinear and quadrupolar short-range interactions is studied within the cluster approximation. Phase diagrams in the (magnetic field, temperature) plane are constructed for different values of quadrupolar interaction. Temperature dependences of thermodynamical functions are obtained at different values of the model parameters.

We show that for those values of the quadrupolar interaction when the system undergoes the temperature phase transition between quadrupolar and paramagnetic phases at zero magnetic field, the external magnetic field not only induces a non-zero magnetization in "paramagnetic" and "quadrupolar" phases, but also can split this transition into a cascade of phase transitions: "quadrupolar" → ferromagnetic → "paramagnetic" phase.

The critical points of different types and the triple points of the system are also discussed.

Creation of K_2LaX_5-Ce^{3+} (X=Cl, Br, I) microcrystals as a model of aggregation processes in lava-like fuel containing materials

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It is known that chemical interactions of nuclear fuel with structural materials of the reactor and backing materials during and after the accident at the Chornobyl' power plant lead to formation of lava-like fuel containing materials (LFCM) with a series of dispersed crystalline inclusions of the $U_zZr_yO_x$, $ZrSiO_4$, $U_{1-x}Zr_xSiO_4$, $FeSiO_4$ types. Possibility for formation of nanocrystalline inclusions in LFCM was simulated by an example of Pb^{2+} ions aggregation in haloid crystalline matrices of different structure [2].

It is known that LFCM contain a small amount of ^{239}Pu, ^{241}Am, ^{244}Cm ions. Their radiation results in formation of different anionic and cationic vacancies, which can both assist the aggregation processes and lead to destruction of the formed aggregates. There arise a question whether the formed aggregates of the $U_zZr_yO_x$, $ZrSiO_4$, $U_{1-x}Zr_xSiO_4$, $FeSiO_4$ type can concentrate in themselves the ^{239}Pu, ^{241}Am, ^{244}Cm ions and transform into submicronic particles under their irradiation.

Embedding of actinoid ions into the matrices based on uranium compounds can be simulated by embedding lantanoid ions into complex crystalline structures based on lanthanum salts. That is so due to a certain similarity between external electron shells of lantanoid and actinoid ions.

We explore the processes of embedding Ce^{3+} ions into microcrystals of the K_2LaX_5 type (X=Cl, Br, I), dispersed in KX (X=Cl, Br, I) matrices. Spectral-luminescent parameters of these crystals confirm a possibility of such embedding. Therefore, a hypothesis can be set up that the crystalline aggregates of the $U_zZr_yO_x$, $ZrSiO_4$, $FeSiO_4$, $U_{1-x}Zr_xSiO_4$ type can serve as concentrators of high-energy α, β, γ-irradiaion sources (^{239}Pu, ^{241}Am, ^{244}Cm, ^{137}Cs).

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Monoclinic elastic and piezoelectric properties of Rochelle salt. Description within the modified Mitsui model with piezoelectric and strictional interactions

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We propose a further modification of two-sublattice Ising model with asymmetric double-well potential (Mitsui model), traditionally used for description of the physical properties of Rochelle salt crystals. In addition to the coupling with the spontaneous shear strain ε_4, which taking into account has been recently proposed [1], the present modification also takes into account the coupling with diagonal components of strain tensor ε_i $(i = 1, 2, 3)$, which arise due to thermal expansion or under action of external pressures which do not affect the crystal symmetry (e.g. hydrostatic). We calculate the related to these strains piezoelectric and elastic characteristics of Rochelle salt. According to the crystal symmetry, most of the calculated characteristics differ from zero only in the ferroelectric (monoclinic) phase. A numerical analysis of the obtained results is performed. In the approximation of zero thermal strains, we find a set of the theory parameters, providing a satisfactory quantitative agreement with the available experimental data for the monoclinic elastic constants c_{i4} and piezomoduli d_{1i}, g_{1i} $(i = 1, 2, 3)$.

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Multiple-factor influence on the interaction of organic solvents with polymeric structures

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A great number of investigations are related with the problem of the interaction in polymer — solvent systems due to its theoretical and practical importance: swelling of polymers determines their mechanical stability; membrane technologies are based on the diffusion through polymers; dissolution of polymers leads to producing of latexes, gels, glues. Nevertheless, till now there is no reliable theory on the interaction in such systems.

The most spread seems to be Flory-Huggins approach, based on Hildebrand theory of regular solutions. According to this approach, the degree of swelling of polymer (or the other characteristics) are proportional to the square of the solubility parameter δ of solvent. However, this approach takes into account only structural factors but not possible chemical interaction, that is why reliable linear relations are obtained only within the limits of separate groups of solvents. Brislow and Watson as well as McGee have introduced the empiric correcting coefficient χ. However, that did not solve the problem. Similarly the attempts of interpretation of these processes using only chemical factors of interaction, for example, donor numbers DN, also lead to unsatisfactory results.

We generalized a large number of data from publications and ascertained that the reliable results may be obtained on the base of the principle of linearity of free energies, that is indicators of the interaction in polymer — solvent systems are considered as the result of the algebraic sum of separate energetic effects. The following equation was found to be effective:

$$\lg X = a_0 + a_1 f(n^2) + a_2 f(\epsilon) + a_3 B + a_4 E_T + a_5 \delta^2 + a_6 V_{\mathrm{M}},$$

where the first two members take into account the influence of polarity and polarizability of solvents, the next two members — possible acid-base interaction and V_{M} is molar volume of the solvent. As a rule, the latter factor has the negative influence on the characteristics of the interaction (the larger size of the molecule the more difficult it penetrates into the structure of the polymer macromolecule). Solvatation factors, on the contrary, promotes the interaction and δ^2 is not significant in the most of cases.

The suggested approach appears to be suitable for generalisation of the results on the extraction of natural polymers-coals.

Electrophysical parameters of metallic nano-particles in dusty plasma systems

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The ionization states of dusty plasma are theoretically investigated in the range of thermodynamic parameters, character for industrial applications: 1500–4500 K, 0.01–1 MPa.

An original approach has been developed for the description of the thermo-ionizational equilibrium, based on the effective cell screening model. The cell volume was used as the spatial scale of charges separation in the dusty plasma. It is determined by the electromagnetic interaction of particles with the electron-ion component of the plasma gaseous phase. It is found by the minimization of the Coulomb contribution to the Helmholtz functional of the dusty plasma. The functional dependence of the individual particle potential on its charge in the plasma medium is investigated in details. The work function has been found to have a maximum in its dependence on nano-particle size. The dependence of particles ionization on the dielectric and electronic parameters of the metal which they are formed from have been obtained for the first time. The Thomas-Fermi approximation was used for the energy dispersion equation of conductivity electrons of the macro-particles.

Practical applications of obtained results to generation and separation of hard-melting metallic particles in plasma reactors are discussed.

Statistical averages of macroparticles electric charge in heterogeneous plasma systems

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For theoretical models and practical applications there is a necessity of an adequate description of Coulomb microinhomogeinity in heterogeneous plasma systems (HPS) which contains high-temperature buffer gas and particles of condensed phase. In statistic equilibrium the Coulomb microinhomogeneities in HPS with polydispersed particles must correspond to the minimum of the Coulomb contribution to the Helmholtz free energy. In the present work based on the statistical model of quasineutral cells of HPS we proposed the way to take into account the dispersion of condensed phase which is based on the minimization of the plasma free energy. Starting from the Kubo principle of the local thermodynamical equilibrium the obtained results can be extended to non-equilibrium systems as well, with relaxation times in regions much less than the existence time of the system.

The size of the electroneutrality domain of HPS basing on the cell model the electrophysical parameters of the system were calculated: charges of dispersed particles, the distribution of self-consistent electric field in the vicinity of individual macroparticles, and the electron concentration in gas phase. For model distribution functions (Gaussian, log-normal, additive) is a computer experiment was performed in order to determine the dependencies of electrophysical parameters on the determining thermodynamical ones. A good correspondence of the data obtained with existing experimental data on the charge particles in combustion plasma products was obtained.

Conformation of linear macromolecules in the real dilute solution in the self-avoiding random walks statistics

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It was proposed a simple model, which introduces a difference of standard free energies of two possible states of neighbor links of polymeric chain in the real solvent at the expense of effects of an interaction "monomer-monomer-solvent". Via the framework of self-avoiding random walks statistics this means, that the internal forces are formed, under the action of which the polymeric chain at its transformation from ideal solvent into the real one decreases its own conformational volume and increases a free energy of conformation. That is why any real solvent with respect to ideal one represents by itself a "bad" solvent. It have been determined the relationships between the states of polymeric chain, its thermodynamical and elastic properties in the ideal and real solvents. It was shown, that the character of changing the thermodynamical and elastic properties of polymeric chain essentially depends upon the ratio of sizes and signs of internal and external forces acting on it starting state in the real solvent. Obtained dependencies were illustrated by calculations.

New look on liquid-vapor coexistence in simple liquids

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In their Monte Carlo study [1] of the phase diagram of hard-core plus attractive Yukawa tail $-\epsilon \exp(\kappa[1-r])/r$ model system, Hagen and Frenkel have shown that no stable liquid phase is possible when the range of the Yukawa attraction is less than approximately one-sixth of the hard-core diameter, i.e. when $\kappa > 6$.

We exploit this finding in a set of theoretical studies of the liquid-vapor coexistence in model simple fluids by using as the reference system the attractive Yukawa potential with $\kappa > 6$. Analytical treatment of such a reference system is available within the mean spherical approximation. The theories where short-range Yukawa attraction was used as the reference system include simple first-order thermodynamic perturbation theory and few first approximations of the collective variables approach. The numerical results for attractive Yukawa potential with $\kappa = 1.8$ that is associated with Lennard-Jones potential are discussed in details and comparison with Monte Carlo data is performed. The possibility to apply the attractive and repulsive Yukawa potentials with $\kappa > 6$ as a reference system to study the liquid-vapor coexistence within a restricted primitive model of electrolyte solutions is outlined as well.

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Relaxation processes and transport phenomena in classical liquids

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The non equilibrium state of liquid is describing by the of generalized common hydrodynamics equations, containing mass currents, impulse and heat, which are obtained based on molecular-kinetic theory. The relaxing currents consist of kinetic and potential parts, determined by single particle $f_1(\vec{x}_1, t)$ and double particle $f_2(\vec{x}_1, \vec{x}_2, t)$ distribution function (DF). The space and time evolution of distribution function are determining by Bogolubov's equations chine [1], which describe with enough rate of dynamic state change completeness of interacting particles. However, these equations in present form directly are not describing non conversional macro processes and, consequently, relaxation processes of system approaches to equilibrium. It is interesting to construct the kinetic equations for the fluids based on Bogolubov's equations chine for non equilibrium DF, describing dissipative processes, which are the aim of present article. Based on method proposed in [2], the kinetic equations for single- and double particle DF, describing non conversional processes in classical liquids. Meanwhile the chain of Bogolubov's equations has been approximated on times less than pairs interactions time and where have been used the condition for particular reduction of initial correlation. The integral parts on the left side of these equations describing the influence of wide scale fluctuations on relaxation processes and are consequences of collective interactions in liquids. Role of interactive parts, obtained only by approximation of pair interactions in right sides of equations, leads to their symmetry destruction relevant to time reflection and ensure describing of dissipative processes. On the base of these initial equations the transport phenomena, elastic and acoustic properties of classical (single, ion, magnetic and electrolyte solutions) liquids have been investigated. The obtained theoretical results satisfactory are corresponding with the existing experimental dates.

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Phase diagrams of Yukawa-Lennard-Jones spin fluids from an integral equation approach

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We develop an integral equation approach to study nonideal Ising spin fluids in the presence of an external magnetic field. In these fluids, the nonmagnetic interactions are modeled by the Lennard-Jones (LJ) potential, whereas the spin exchange integral is presented in the Yukawa (YK) form. The calculations are carried out on the basis of the Duh and Henderson closure with a specific Duh-like partitioning of the full potential. The coupled set of the Ornstein-Zernike equation, the closure and the external field constraint are solved using an efficient numerical algorithm. The phase diagrams are obtained for a wide range of the external field and parameters of the interaction potential. As is demonstrated, the changes in the ratio for the strength of YK magnetic to LJ nonmagnetic interactions and the screening YK radius can lead to different types of the phase diagram topology. They are characterized by the existence of critical, tricritical, critical end, and triple points related to transitions between gas, liquid, para- and ferro-magnetic states. Under special van Laar conditions, an unsymmetrical tricritical point is found additionally. Such a complexity with respect to simple LJ fluids is explained by a coupling between spatial and spin degrees of freedom. It is shown that the theory leads to accurate description of the complicated phase diagram behavior which agree well with simulation data obtained by the Gibbs ensemble and multiple-histogram reweighting techniques.

This work was supported by the Austrian Fonds zur Förderung der wissenschaftlichen Forschung, project No P15247.

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Molecular dynamics simulation of melting and crystallization

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Molecular-dynamic simulations have been fulfilled for argon for different border conditions: periodical, ideal walls or isothermal walls, big box with ideal or isothermal walls and big box with several mirror walls. Three mirror walls, which cross in one corner, allow multiplying by eight the effective quantity of atoms in system. Pair atom interaction was described by the well-known Lennard-Jones potential, which is usually used for argon.

Some points are known which obstruct to dynamic modeling of crystallization. Border conditions influence essentially the results. A large computer time is necessary to reach equilibrium states. It is practically impossible to study nucleation at cooling because of small sizes of system in consideration. Therefore it is important to know exactly how results of calculations depend on the border conditions and how effective size of systems influences the melting temperature and character of phase transition.

We have found that hysteresis of melting and crystallization always takes place and the temperature of crystallization depends on the lifetime of system in the liquid state after melting. The melting temperature increases whereas the number of atoms increases. Periodical conditions are most favorable for crystallization. Free nanocrystals or liquid nanodroplets are mobility enough. As a rule, drops after crystallization consist of several large crystal clusters with different orientations. Ordering changes continuously from one crystal cluster to other or from the crystal clusters to liquid part of the droplet during crystallization or melting. Free crystals fall to pieces after beginning of simulation as a rule if their atom structure is not in compliance with the face-centered cubic lattice.

This work was supported in part by SFFR of Ukraine (project No. 2.7/418).

Phase behavior of ion-asymmetric fluids

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In this report we address an issue of the phase behavior of ionic fluids using the functional integration methods. We consider a case of the primitive model describing a binary mixture of equisized hard spheres that carry positive and negative charges of different magnitude. Starting from the Hamiltonian we obtain the functional representation of the grand partition function in terms of the two types of fluctuating variables (collective variables) describing fluctuations of the total number density and charge density, respectively. Based on this functional we study the gas-liquid critical point. The results obtained are compared with those found by other theoretical technique as well as by computer simulation methods.

Influence of the InAs/GaAs nanoheterostructure growth temperature on the spectral standing of a maximum of a curve of photoluminescence at InAs quantum dot

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Nowadays, significant interest is attracted by heterostructures with quantum dots (QDs). It is connected with an opportunity to expand the optical range of emission and stimulated by modern optoelectronics needs in effective solid-state emitters (lasers).

The process of formation of InAs QDs on singular and vicinal GaAs surfaces by the method of molecular beam epitaxy in the InAs/GaAs system is composed of two stages. In the first stage, the growth of an InAs pseudomorphic strained layer occurs. After the critical thickness of 1.5-1.7 ML (monolayer) has been reached, the second stage begins. The latter, according to the Stranski-Krastanow growth model, comprises a spontaneous decay of the pseudomorphic layer into a system of crystal islands (QDs) and a wetting InAs layer about 1 ML in thickness. Varying the growth temperature, one can affect the degree of deformation of an epitaxial layer deposited onto a substrate. Ultimately, it will cause a modification of the energy spectrum of current carriers in the QD, i.e. a variation of optical properties of heterostructures with QDs.

This work aims at calculating the energy of the basic optical transition within a coherent-strained QD and analyzing the dependence of this energy (or the relevant frequency) on the growth temperature and the dimensions of a QD.

It is established that both with increase of growth temperature, and with increase of the sizes of a quantum dot an optical gap diminishes. The character of the dependence of the transition energy E on the QD growth temperature T is governed by the T-behavior of its components: the increase of the growth temperature stimulates the raise of electron and hole energy levels in the QD and a reduction of its energy gap width. The rate, at which the energy gap diminishes, substantially exceeds the rates, at which the electron and the hole ground state energies in the QD raise.

Formation of the $n - n^+$ junctions caused by self-organizational effects in a crystal with dot defects

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Exterior influence (laser exposure, the irradiation by beams of particles etc.) creates high concentrations of dot defects (an interstitial atoms and a vacancy) in solid states. The interaction of dot lattice defects with self-consistent deformation field, caused by dot defects, results in a formation of ranked defect-deformation (DD) structures: clusters and periodic structures. The reason of the appearance of non-uniform deformation, which results in local change of the band spectrum, is the presence of DD-structures. As a consequence, the spatial redistribution of electrons takes place, which gives birth to the electrostatic potential. To find the electron density and the electrostatic potential, it is necessary to solve self-consistently the following system of equations:

1) the stationary Schrödinger equation;
2) the equation of mechanical equilibrium;
3) the equation which determines the concentration of electrons;
4) the Poisson equation used to determine the electrostatic potential;
5) the equation of the determination of the chemical potential.

The criterion of the appearance of an $n-n^+$ junction is concentration of lattice defects. At concentration of defects $n_{d0} < n_{dc1}$ (n_{d0} is the medial concentration of defects) the processes of self-organizing of defects are absent and, accordingly, a $n - n^+$ junction is absent.

Within the interval of concentration of defects $n_{dc1} < n_{d0} < n_{dc2}$ the clusters in a crystal are formed, which are the reason of non-uniform deformation. In a result, there is a shortage of electrons in of one part of a crystal, and surplus – in another. Thus, the double electrical layer is formed in a crystal with dot defects.

At medial concentration of defects $n_{d0} > n_{dc2}$ the defect periodic structures are formed. Accordingly, redistribution of electrons will have periodic character, and the sequentially joint $n - n^+$ junctions appear.

Bose-gas with an arbitrary dispersion law in a trap

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In the present work, a simple technique based on the ideal Bose-gas theory is proposed. We consider the dispersion law of an arbitrary form $\varepsilon = f(|\mathbf{p}|)$, where ε stands for energy and $\mathbf{p}$ stands for the momentum of a particle. In order to give a more generalized description, we study the system in D dimensions. For brevity, we write $|\mathbf{p}| = p$.

One can calculate the energy as follows:

$$E = \frac{(2s+1)\Omega_D}{(2\pi\hbar)^D} \int_{\varepsilon_{\min}}^{\infty} \left. \frac{p^{D-1}}{f'(p)} \right|_{p=f^{-1}(\varepsilon)} \frac{\varepsilon \Pi(\varepsilon)\, d\varepsilon}{e^{(\varepsilon-\mu)/T} - 1}$$

with f^{-1} denoting the inverse function. Here, s is the spin of a particle, T is temperature, Ω_D is the full D-dimensional hyper-angle. The chemical potential μ is obtained from the condition that the number of particles in the system is fixed. The function $\Pi(\varepsilon)$ is determined by the domain accessible for the particle when the trapping potential is turned on. This function is obtained in the quasi-classical approach [1] by integrating the space variables within the classical turning points. In many cases, $\Pi(\varepsilon) \propto \varepsilon^{\delta}$, where the exponent δ is defined by the form of the trap. This fact gives the possibility to treat the system under consideration to be in an effective dimension (usually fractional) other than the original one.

Using the energy one can then calculate other thermodynamic functions. A separate attention should be paid to the Bose-condensation phenomenon appearing at the temperatures $T < T_c$ such that $\mu(T_c) = 0$.

Several particular cases of the dispersion law are of the special physical interest: (i) Power dispersion law $\varepsilon = \alpha p^{\beta}$. This dependence generalizes an ideal Bose-gas ($\alpha = 1/2m$, $\beta = 2$), ultrarelativistic or phonon gas ($\alpha = c$, being the speed of light or sound, respectively, $\beta = 1$), etc. (ii) Relativistic Bose-gas $\varepsilon = \sqrt{m^2c^4 + p^2c^2}$. (iii) Elementary excitation spectrum in the Bogoliubov's form $\varepsilon = \sqrt{ap^4 + bp^2\,\nu_p}$ with ν_p being the Fourier transform of the interatomic potential, $\nu_p = \text{const}$ for the hard spheres model, $\nu_p \propto 1/p^2$ for the Coulomb interaction, etc., cf. also [2].

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Phase transformations in Ti-alloy VT22 induced by pulse magnetic field

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The effect of a weak pulse magnetic field (PMF) on a phase state in Ti-5Al- 5Mo-5V-1Cr-1Fe alloy (VT22) was investigated by X-ray and optical metallographic methods. Different phase states were realized in alloy by special thermal annealing. One- and two-phase samples were undergone to a pulse magnetic field influence with an amplitude up to $H = 10^6$ A/m and a frequency on the range 1–50 Hz. The correlation of fronts for pulse time was 1:10. The appearance of the second α-phase particle was observed in 100% β-phase sample after pulse magnetic field and the portion of α-phase was increased with frequency. In two-phase samples the ratio of phase was change and the pick width on the X-ray picture was increased that indicated the rise on stresses in alloy under action PMF. In our opinion, the effect of PMF have been consisted in an ordering of magnetic moments of iron atoms along the direction of magnetic field which leads to the appearance of the angular moments, and, as result the mechanical stresses in an atom vicinities. Probably, the particles of new phase were generated in places where magnetic atom clusters were formed. PMF frequency with the steep impulse form defines the accumulation rate of mechanical moments. The rate increase tends to rise the adiabatic degree of the exposure process and the input energy into material rise. The relaxation of the energy in the alloy was realized by an increase of stresses and generation of second phase particles.

On the theory of current states in superconducting junctions of SNINS type

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It is carried out a investigation of the current states, which can exist in an SNINS junction (where S – superconductor, N – normal metal, I – insulate) under supposition that the layer's thickness to be arbitrary and temperature to be close to critical.

The behavior of the order parameter near the NS interface in an SNINS junction is considered. For this linear integral equation, which is valid near the superconductor-normal metal interface is obtained and researched. With aid the linear integral equation and within the method quasiorthogonality to asymptotics [1] the boundary condition for the Ginzburg-Landau equation is obtained. The boundary condition involves a barrier transparency, an interlayer thickness, a temperature, a phase difference. If thickness of the normal layer $d \gg \xi_0$ (ξ_0 – coherence length) the boundary condition is not dependence on a phase difference.

Taking into account an influence current on the spatial behaviour of the order parameter the Ginzburg-Landau equation is solved. It is shown that the presence of the current in an junction reduces value of the order parameter in comparison with currentless case.

Main result of this investigate is the formula for the current states in an SNINS junction for arbitrary thickness of the normal layer. Both current phase and current-thickness relations are shown graphically. As a result one can see that dependence of the current density on the phase difference between the backs of the junction is strongly nonsinusoidal for thin ($d \ll \xi_0$) the normal metal layer at high the barrier transparency.

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To kinetics of emitters of electromagnetic field taking into account nonequilibrium correlations

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A liquid consisting of two-level emitters of electromagnetic field is considered. Emitters are described with the quasispin Dicke type model. Hamiltonian of the system encludes contributions of free photons $\hat{H}_b$, free liquid $\hat{H}_s$ and liquid-photons interaction $\hat{H}_{sb}$:

$$\hat{H}_s = \hat{H}_{s0} + \hbar\Omega_0 \hat{R}_0^z, \quad \hat{H}_{sb} = \frac{1}{\sqrt{V}} \sum_k g_k \left(\hat{R}_k^+ c_k + h.c. \right),$$

where term $\hat{H}_{s0}$ corresponds to translational degrees of freedom of the liquid (Ω_0 is own frequency of emitters) . Operator $\hat{H}_{sb}$ describes small emitter-photon interaction and contains Fourier transformed quasispin density $\hat{R}_k^l$ (function g_k defines intensity of interaction). In the present work the stage of the evolution of the system was studied when translational degrees of freedom of the liquid and photon subsystem are in equilibrium states with temperatures T_s, T_b respectively. The emitters subsystem is describes with averages values $R_k^l(t)$ of quasispin densities $\hat{R}_k^l$. The Bogolyubov functional hypothesis was placed in the basis of consideration. For statistical operator of the system $\rho(R(t), T_s(t), T_b(t))$ an integral equation was constructed, which is solvable in a perturbation theory in g_k. This has been done with accounting of the boundary condition of the complete spatial correlation weakening. As a result closed system of time equations for parameters $R_k^l(t)$, $T_s(t)$, $T_b(t)$ were obtained. A possibility to take into account in the reduced description (RD) of the system emitter-emitter correlations was investigated too. This RD was built on the base of the following approach: the RD theory without nonequilibrium correlations as independent RD parameters but with a random initial state leads with the help of the corresponding averaging to the RD theory taking into account nonequilibrium correlations (S. Peletminskii, A. Sokolovsky, Yu. Slyusarenko).

This work was supported by SFFR of Ukraine (project No. 2.7/418) and in part by INTAS (project No. 00-577).

Vibrational properties of CsD_2PO_4

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Lattice dynamics of CsD_2PO_4 was simulated both in monoclinic $P2_1/m$ paraelectric and $P2_1$ ferroelectric phases at ambient pressure. The phonon dispersion relations in the entire Brillouin zone, velocities of ultrasonic waves, density of phonon states, specific heat, mean squared displacements of atoms and anisotropic thermal parameters were calculated in the quasi-harmonic approximation within the framework of semi-phenomenological atomistic model. The model takes into consideration the Coulombic, short-range and covalent interactions. The deuteron-oxygen interactions within the hydrogen bonds were evaluated by means of empirical potential.

Results of simulation agree well with the experimental data. The eigen-vector analysis of phonon modes enables us to interpret properly the very complicated Raman and IR spectra.

The experimental IR spectra reflected from the monoclinic (a, c) plane provide only a qualitative information because the dipole moments of B_u phonon modes can be oriented anyhow in (a, c) plane. Therefore, the correct information about the frequencies of B_u TO modes cannot be obtained within the commonly used experimental IR methods. Simulated polar diagrams of B_u mode frequencies in (a, c) plane allow establishing the values of pure TO and LO mode frequencies and the direction of dipole moments of polar phonon modes.

Self-organization process evolving in accordance with Hopf bifurcation

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Behavior of the simplest self-organized system is known to reduce to standard picture of thermodynamic transition where an effective potential has a single minimum. Much more complicated situation takes place for deterministic systems displaying regime of the strange attractor which can not be corresponded with some potential. In this work, we consider intermediate case when effective potential possesses degenerate minima that correspond to a limit cycle. As is known such transition evolves in accordance with Hopf bifurcation [1].

We start with the Lorenz system [2]

$$\begin{cases} \dot{\eta} = -\eta + h, \\ \sigma\dot{h} = -h + \eta S, \\ \varepsilon\dot{S} = (S_e - S) - \eta h \end{cases} \tag{1}$$

where η, h and S are an order parameter, its conjugate field, and a control parameter, respectively; overdot stands for the time derivation, S_e is a driven force; multipliers $\sigma \equiv \tau_h/\tau_\eta$ and $\varepsilon \equiv \tau_S/\tau_\eta$ determine relations of characteristic time scales. We study the most interesting case $\tau_h/ \ll \tau_\eta, \tau_S$ when $\sigma \ll 1$, so that $h = \eta S$. Moreover, in accordance with catastrophe theory, we introduce an external field $f_e = A + B\eta + C\eta^2 + D\eta^3 + F\eta^4$ where A, B, C, D, and F are theory parameters. Then, governing equations take the form

$$\begin{cases} \dot{\eta} = -\eta(1 - S) + f_e, \\ \dot{S} = \varepsilon^{-1}[S_e - S(1 + \eta^2)]. \end{cases} \tag{2}$$

We find analytically the conditions of stability of the limit cycle and solve numerically the system (2) to build up related phase portraits.

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Band electron spectrum and thermodynamical properties of the pseudospin-electron model with tunneling splitting of levels

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The pseudospin-electron model with tunneling splitting of levels is considered. Generalization of dynamical mean-field method for systems with correlated hopping was applied to the investigation of the model.

Within the alloy-analogy approximation the numerical investigations were conducted and electron spectrum was calculated. The dependences of the electron concentrations and average pseudospin values on chemical potential, asymmetry field and tunneling probability were obtained. It was shown, that in alloy-analogy approximation the model possess the first order phase transition to ferromagnetic state with the change of chemical potential and second order phase transition with the change of temperature.

Charge and magnetic states for Hubbard model on a triangular lattice

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The Hubbard model for small size clusters is investigated. Using an exact diagonalization method and a Hubbard operators formalism the eigenvalues and eigenstates for the Hubbard model are determined. By means of the Green's function method the electronic, magnetic and spin susceptibilities are calculated and their behavior at low temperatures is investigated for the chain with $N = 2$ and $N = 3$ periodic boundary conditions (two- and three-site clusters, respectively). The temperature behavior of susceptibilities is investigated for both center and edge of the Brillouin zone. If at given concentration the ground state is polarized, susceptibilities diverge following the Courie law and system is transformed to the ferromagnetic state at $T = 0$. It is shown that the geometrical frustration influences on a system behavior. Obtained results are in good agreement with those received for the Heisenberg model (which is considered in three-site cluster case for comparison).

Stochastic storage model and phase transitions

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The most frequently used class of stochastic process modelling physical phenomena at mesoscopic description level is that based upon Fokker-Plank equation, that is on the diffusive model essential feature of which are (infinitively) small jumps of the random value. Because of that the description of such problems as, e.g., phase transitions, where the system is to overcome some finite potential barrier, seems self-contradictory from the outset.

We suggest the alternative stochastic description of physical systems based on the easy-to solve stochastic storage model in which the jumps of the stochastic process need not to be small. From the very beginning the kinetic coefficients of the underlying Markovian process essentially disobey the detailed balance principle, so such process could be suitable for describingessentially nonequilibrium systems. The class of models considered has as natural solution the probability distribution function as γ-distribution on the contrast to the Gausians of the Fokker-Planck scheme. Such γ-distributions were proved to be promising in describing characteristic feature of non-additive statistics (such as Tsallis statistics).

The generalization of the base scheme of stochastic storage process is proposed following the lines leading to the generalization of the ordinary Fokker-Planck equations to higher derivative terms, On the contrast to the Gaussian processes where the development is performed in series over small parameter of the jump value, more appropriate to the storage models series are considered. The kinetic potential generalizing the classical storage model is introduced.

For noise-induced phase transitions (e.g. Ferhulst model) the reliable results can be obtained for the simplest (linear) forms of the escape function.

Microscopic derivation of the hydrodynamics equations for the superfluid fermi-system

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In the weakly-nonequilibrium states equation of hydrodynamics is the important instrument of description of the quantum liquids. As known, the phenomena of superconductivity and superfluidity are deeply family. Property of the nondissipative currents states, that arises up as a result of phase transition to more well-organized state, unites them [1]. At phenomenological level two-fluid hydrodynamics for superfluid He-4 was built Landau [2]. At microscopic level these equations was derived by Bogolubov [3]. Hydrodynamics of superfluid fermi-system was built in the work of Svidzynsky and Slusarev [4]. By a starting point for construction of hydrodynamic equations in works [3], [4] there is the system of equations of motion for correlations functions.

For transition to equations of hydrodynamics the expansion of equations of motion in terms of a small parameter was executed. That a small parameter is inculcated formal is the noticeable lack of these works. In work [3] it is the so called "parameter of homogeneity". In work [4] it is Plank constant which, obviously, it was possible to put to even unit.

In this work, where following chart of work [4], starting from the first principles of statistical mechanics the equation of two-fluid hydrodynamics of superconductor in ideal approximation was derived. Thus, writing down equation of motion for correlations functions in a dimensionless form, it is succeeded to select a small parameter. It is equal to the attitude of the length of coherence (which is to the order of 10-4 cm.) toward the characteristic length which macroscopic quantities change on (as the middle number of particles, impulse and others like that). The expansion in terms of a small parameter coincide with the expansion in terms of a gradients of the macroscopic quantities.

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Influence of external factors on dielectric permittivity of Rochelle salt: humidity, annealing, electric field, uniaxial pressure

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We study the influence of humidity, thermal annealing, longitudinal and transverse electric fields, uniaxial pressures. external factors on the 1 kHz dielectric permittivity of Rochelle salt crystals.

Essential differences in the permittivity of dessicated and wet samples of Rochelle salt are observed, especially in the ferroelectric and upper paraelectric phases. Thermal annealing is shown to decrease the upper transition temperature and increase the peak value of permittivity. Those effects are attributed to annealing of polar defects in samples, which action is similar to that of longitudinal electric field (internal bias field).

The longitudinal electric field, being the field conjugate to the order parameter, acts in accordance with well-known phenomenological predictions: decreases the peak values of permittivity and widens the ferroelectric region. The obtained data are interpreted in the framework of the Landau theory; values of the Landau coefficients are determined. Straighforward attempts to describe the field effects within the modified Mitsui model [1] have shown that near the upper transition point the internal effective fields are much lower than the applied external ones, possibly due to the perceptible conductivity of Rochelle salt crystals above the room temperature. No such effect is found near the lower transition point.

The transverse field does not affect the transition temperatures (within the measurement error), but essentially changes the peak values of permittivity.

Uniaxial pressures applied the main crystallographic directions of Rochelle salt crystals are shown to decrease the peak values of permittivity and shift the peak temperatures. These data are interpreted within the Landau theory.

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The Bogolyubov functional hypothesis and Zubarev's method of nonequilibrium statistical operator

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Reduced description of a system with the help of average values of operators $\hat{P}_m$ has been discussed in the absence of time dependent external field. Starting point of the consideration is the Bogolyubov functional hypothesis

$$\rho(t) \xrightarrow[t\gg\tau_0]{} \rho^{as}(t) \equiv \rho(P(t,\rho_0)), \qquad Sp\rho(P)\hat{P}_m \equiv P_m \tag{1}$$

($\rho_0 \equiv \rho(t=0)$), where the last formula defines reduced description parameters (RDP) $P_m(t,\rho_0)$. Asymptotic statistical operator (SO) of the system $\rho^{as}(t)$ satisfies the Liouville equation for $t >> \tau_0$. Assuming that this equation for $\rho^{as}(t)$ is valid for $t \in (-\infty,+\infty)$ we define the RDP for non-physical times $t \leq \tau_0$. After this procedure time equation for the RDP $P_m(t,\rho_0)$ is true for $t \in (-\infty,+\infty)$. Quasi-equilibrium SO of the system is defined by the formulae

$$\rho_q(F) = \exp\{\Phi(F) - \sum_m F_m \hat{P}_m\}, \qquad Sp\rho_q(F) = 1. \tag{2}$$

Let us introduce functions $Y_m(P)$, which are mutually reciprocal with functions $P_m(0,\rho_q(Y))$. Using the functional hypothesis (1) it has been proved that for $t \in (-\infty,+\infty)$

$$\rho^{as}(t) = \lim_{\varepsilon\to+0}\rho(t,\varepsilon), \rho(t,\varepsilon) \equiv \varepsilon\int_0^{+\infty} dt' e^{-(i\mathbf{L}+\varepsilon)t'}\rho_q\left(Y\left(P\left(t-t',\rho_0\right)\right)\right)$$

($Sp\rho^{as}(t)\hat{P}_m = P_m(t,\rho_0)$; $\mathbf{L}$ is the Liouville operator; all values dependent on ε are shown). The obtained expression for SO $\rho^{as}(t)$ is close to proposed by Zubarev in his method of nonequilibrium SO (NSO). However, in the NSO method functions $F_m(P)$ defined by the formula $Sp\rho_q(F(P))\hat{P}_m = P_m$ are used instead of the functions $Y_m(P)$. Our dependence of SO $\rho(t,\varepsilon)$ on ε corresponds to one proposed by Auslander and Kalashnikov.

This work was supported by SFFR of Ukraine (project No. 2.7/418) and in part by INTAS (project No. 00-577).

Equations of nonlinear plasma electrodynamics with nonequilibrium correlations of the field

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Construction of nonlinear motion equations for electromagnetic field and its correlations is important modern problem of the great interest for electrodynamics of continuous media. Nonequilibrium correlations must contribute to the mentioned equations alongside with the more standard nonlinear terms. The problem has been investigated with the help of the Bogolyubov reduced description method based on the functional hypothesis. This method allows to construct a closed system of Markovian time equations for reduced description parameters which in our consideration are averaged electromagnetic field and all its correlations (centered moments). The method leads to an integral equation for statistical operator of the system solvable in a perturbation theory in small electromagnetic interaction. In the present work the medium (plasma) is assumed to be in equilibrium. The mentioned integral equation was built in an usual way with the help of the boundary condition of the complete spatial correlation weakening. Statistical operator of the system was calculated up to the third order in small parameters that gives time equations for reduced description parameters, which include among others standard contributions of the nonlinear optics. The small parameter of the developed theory is the ratio of the plasma frequency and characteristic frequency of the main processes in the plasma. The obtained closed system of time equations for the field correlations in homogeneous isotropic equilibrium plasma takes into account a spatial dispersion that is substantial for the the third order terms. Due to expansion in interaction the time dispersion is taken into account in structure of kinetic coefficients (conductivities) that leads to the equations in a Markovian form. For all correlations moments waves of correlations were investigated close to equilibrium. The waves for correlators of even number of fields exist in a homogeneous isotropic case too. An analysis of the nonlinear terms has shown that the higher correlations are source for lowest and vice versa. The microscopic expressions for all linear, binary and triple conductivities are obtained through parameters of the medium.

This work was supported by SFFR of Ukraine under project 2.7/418.

Kinetics of a system in nonequilibrium medium taking into account influence of the system on medium

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Kinetics of a system s in a medium b is considered. The state of the systems s and b are described with the variables $\gamma_n(t)$ and $\eta_a(t)$ correspondingly. The problem is solved with help of the Bogolyubov reduced description method based on the functional hypothesis. The connected set of equations for the mentioned reduced description parameters has been derived as a result

$$\partial_t \gamma_n(t) = M_n(\gamma(t), \eta(t)), \quad \partial_t \eta_a(t) = L_a(\gamma(t), \eta(t)). \tag{1}$$

The following model was placed in the basis of the consideration

$$\begin{aligned} &\mathbf{L} = \mathbf{L}_s + \mathbf{L}_b + \mathbf{L}_{sb}, \quad \mathbf{L}_{sb} \sim \lambda, \quad \lambda << 1; \\ &\mathbf{L}_s \hat{\gamma}_n = -i \sum_{n'} c_{nn'} \hat{\gamma}_{n'}, \quad \mathbf{L}_b \hat{\eta}_a \sim g, \quad g << 1 \end{aligned} \tag{2}$$

($\hat{\gamma}_n$, $\hat{\eta}_a$ are operators corresponding to the variables $\gamma_n(t)$, $\eta_a(t)$). Here $\mathbf{L}_s$, $\mathbf{L}_b$ are the Liouville operator of subsystems s, b and $\mathbf{L}_{sb}$ describe a small interaction s and b. Relation between $\mathbf{L}_s$ and $\hat{\gamma}_n$ shows that for system s the Peletminskii-Yatsenko model of nonequilibrium processes has been used. The last estimation in (2) shows that variables of the medium $\eta_a(t)$ are slow ones. Functions $M_n(\gamma, \eta)$, $L_a(\gamma, \eta)$ were calculated in a perturbation theory in λ, g. Dependence of $L_a(\gamma, \eta)$ on γ_n describes an influence of the system s on the medium b. For statistical operator $\rho(\gamma(t), \eta(t))$ of the system $s + b$ an integral equation solvable in the described perturbation theory was obtained. This has been done with the help of the boundary condition of the complete spatial correlation weakening. A possibility to take into account in the reduced description of the considered problem nonequilibrium correlations was investigated too. The obtained results were applied to kinetics of electrons in a crystal as a phonon medium.

This work was supported by the SFFR of Ukraine (project No. 2.7/418).

Relaxation phenomena for electrons in crystal beyond the Landau approximation

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The present work is based on obtained by us kinetic equation for electrons in crystal weak interacting with equilibrium phonon subsystem. It was done without any assumption about weak non-uniformity of the state of the system. Relaxation of the average velocity of electrons u_l to zero and temperature T to temperature of the phonons T_0 has been investigated. In the considered situation contrary to number of electrons their energy and momentum are non-conserved values. At first this problem was studied by Landau for temperatures of two component plasma. Landau used in his solution of the problem the Maxwell distributions with time dependent temperatures as nonequilibrium distribution functions. However, these functions do not satisfy his kinetic equations. The purpose of the present work is to find real nonequilibrium distribution function and to study on this base the relaxation phenomena. The consideration is based on the Bogolyubov functional hypothesis with values $T(x,t)$, $u_n(x,t)$ and $n(x,t)$ as reduced description parameters ($n(x,t)$ is density of electrons). This leads to a generalization of the Chapman-Enskog method. Kinetic equation for electrons at the reduced description was solved in a perturbation theory over $u_n,\ T-T_0 \sim \lambda$ ($\lambda << 1$) and gradients $\nabla_l u_n,\ \nabla_l T,\ \nabla_l n \sim g$ ($g << 1$). In the spatially uniform case linear relaxation is described by solution of the eigenproblem for collision integral. Necessary eigenfunctions was calculated with the help of expansion in a series over the Sonin polynomials. It was established that 3-polynomials approximation gives corrections to the Landau theory. Nonlinear relaxation equations are obtained in the developed theory in the higher order of the perturbation theory in λ. The influence of non-uniformity of the system on relaxation phenomena was investigated too. It was done partially up to the Burnett terms. It is possible in the developed theory because the kinetic equation for electrons takes into account influence of non-uniformity of electron state on electron-phonon collisions.

This work was supported by SFFR of Ukraine (project No. 2.7/418) and in part by INTAS (project No. 00-577).

To kinetics of two-zone semiconductor taking into account electron-phonon correlations

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The simplest model with two types of electrons (from valent and conductive zone) interacting with longitudinal optical phonons is considered. It is neglected with electron spin and phonon polarization effects. Energy of an electron is given with a square function of the wave vector. Electron-phonon interaction was chosen in the Frohlich model with $\hat{H}_{\rm int}$, which is linear in operator of the phonon field $\hat{\varphi}(x)$ and operator of the Wigner electron distribution function $\hat{\rm f}_{\alpha\alpha'}(k,x)$ (the corresponding phonon operator $\hat{\rm n}(q,x)$ is defined through $\hat{\varphi}(x)$). We started from the reduced description (RD) of the system given by the electron and phonon Wigner distribution functions ${\rm f}_{\alpha\alpha'}(k,x,t)$, ${\rm n}(q,x,t)$ and averaged phonon field $\varphi(x,t)$. As a result a closed system of equations for these variables was obtained. The next stage of the present work is to include in the set of RD parameters not only the mentioned variables but some their binary correlations too. This RD was built on the base of idea: the RD theory without nonequilibrium correlations as independent RD parameters but with a random initial state leads with the help of the corresponding averaging to the RD theory taking into account nonequilibrium correlations (S.Peletminskii, A.Sokolovsky, Yu.Slyusarenko). This idea gives the following system of equations for RD parameters $\eta_a(t)$ (i.e. for ${\rm f}_{\alpha\alpha'}$, n, φ) and for the corresponding binary correlations $g_{aa'}(t)$

$$\partial_t \eta_a = e^{A(g)} L_a(\eta)\,,\ \partial_t g_{aa'} = e^{A(g)} \sum_{a''} \left(g_{aa''} \frac{\partial L_{a'}(\eta)}{\partial \eta_{a''}} + (a \leftrightarrow a') \right)$$

($A(g) \equiv \frac{1}{2} \sum_{aa'} g_{aa'} \frac{\partial^2}{\partial \eta_a \partial \eta_{a'}}$). Ignatyuk and Morozov have investigated the mentioned reduced description at $\varphi(x,t) = 0$ and for spatially uniform case but with average value of $\hat{H}_{\rm int}$ as an additional RD parameter. The last our equation gives a very close related theory if we restrict ourselves with correlations $\hat{\varphi}(x)$ and $\hat{\rm f}_{\alpha\alpha'}(x)$.

This work was supported by SFFR of Ukraine (project No. 2.7/418) and in part by INTAS (project No. 00-577).

Some features of metal cerium asymptotical behavior

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The thermodynamic behavior of the basic characteristics of metal cerium stability on the stability border , in the neighborhood of the critical point is considered.The relations between critical exponents of isodynamic variables (the IV's):

$$\left(\frac{\partial T}{\partial S}\right)_P \sim \tau^{\alpha},\ \left(-\frac{\partial P}{\partial V}\right)_T \sim \tau^{\gamma},\ \left(\frac{\partial T}{\partial V}\right)_P \sim \tau^{\mu}$$

and adiabatic variables (the AV's):

$$\left(\frac{\partial T}{\partial S}\right)_V \sim \tau^{\alpha_1},\ \left(-\frac{\partial P}{\partial V}\right)_S \sim \tau^{\gamma_1},\ \left(\frac{\partial T}{\partial V}\right)_S \sim \tau^{\mu_1},$$

where $\tau = \frac{T-T_c}{T_c}$ have been obtained using only thermodynamic stability conditions, without any hypotheses.

It is investigated the conditions of turning these expressions into equalities. They are determined by relations between μ and μ_1 .It is shown that the equalities $\alpha+\gamma=2\mu$, $\alpha_1+\gamma_1=2\mu_1$ are fulfilled for cerium for $\mu>\mu_1$. Using the model and experimental data enables to obtain $\alpha=\gamma=\mu=1$, $\alpha_1=\gamma_1=\mu_1=0$.

It is shown, that the supercritical transition curve (a curve of the lowered stability, quasispinodal) on the $P-T$ diagram is the straight line. For cerium this fact enables to make the conclusion that the straight phase equilibrium line continuously passes to the supercritical transition line. It causes the performance of symmetry conditions between critical exponents $\alpha=\alpha'$, $\gamma=\gamma'$.

Thus, the investigation of the asymptotical behavior of the metal cerium, connected with feature of the phase equilibrium line, carried out by the theory of thermodynamic stability method, leads to the conclusions:

a) it is enough to know 2 exponents - one for AV and one for IV- to examine of cerium asymptotical behavior;

b) the symmetry conditions between critical parameters are satisfied.

The critical region thermodynamics of some statistical models

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Successes of the modern theory of critical phenomena have been connected with the fundamental conclusions about the critical state nature and existence of the class of systems, for which both the scaling law hypothesis and universality one are fulfilled. From this point of view real systems and consistent models contradicting to above-mentioned hypotheses are the problem of great importance. The 6-vertex Lieb model and the hard squares model, in which scaling law hypothesis is violated, and Baxter model and Ashkin-Teller one, in which universality hypothesis is violated, are such models. This work is dedicated to critical properties examination of Ashkin-Teller model and hard squares model [1]. We have analyzed the behaviour of the whole set of stability characteristics (adiabatic and isodynamic parameters) in the critical region and have determined critical behaviour types for theses models on the basis of the thermodynamic method of investigation of one-component system critical state. The method is based on the introduction of constructive critical state definition and on the stability examination of critical state. It leads to existence of four types of critical behaviour [2]. The following conclusions have been made:

– the violation of the scaling law hypothesis in the hard squares model is caused by the realization of different behaviour types in subcritical and supercritical regions;

– the violation of the universality hypothesis in Ashkin-Teller model is concerned with two different behaviour types depending on a value or continuum of values of the interaction parameter.

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Glauber dynamics of spin models with different types of competing interactions

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Glauber dynamics of a spin-glass model with essential short-range interactions (first coordination sphere with distribution -aK, K and with a Gaussian distribution of interaction parameters) and weak long-range interaction is investigated within the symmetric replica approach. A system of equations for the linear responses of magnetization and spin-glass parameter within a two-site cluster approximation for the short-range interactions and within linear approximations for the long-range interactions is derived. In the spin-glass region the imaginary part of susceptibility has a high temperature peak (beginning of glass phase) and a low temperature peak. Influence of long-range interactions and random internal fields on the phase diagram and dynamic characteristics of model is studied. Applicability of the theory for description of relaxation properties of the $Rb_{1-x}(NH_4)_xH_2PO_4$-type proton-glasses is discussed.

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Influence of electrostatic interactions on pressure of the electrolyte solution in a porous medium

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The free particles penetration from solution into porous matrix is the peculiarity of the contact of electrolyte solution with porous media. In the study of such systems it is necessary to take into account the thermodynamic equilibrium condition for particles in solution and in pores. This condition leads to the interdependence of the particles densities in the both phases.

A two-phase spatially inhomogeneous system of point-like particles of the ion-dipole mixture in porous media with a sharp interfacial plain is considered as a model of the theoretical description of the contact of an electrolyte solution with porous media. We used the system of replica nonuniform Ornstein-Zernike equations for the description of screening effects of electrostatic interactions. The expressions for two- and one-particle screened potentials have been obtained as the result of the solution of this system. Their asymptotics in the case of long interparticle distances are studied. The influence of the matrix porosity onto the effective interparticle interactions in the case of low ionic dilution is investigated as well [1]. The thermodynamic equilibrium condition is used to study the density distribution of electrolyte particles in pores. The adsorption of ions on a porous silica glass surface SiO_2 with admixtures of Na_2O is calculated for the particular case of the NaCl solution in water. It is shown that the matrix ionization has a significant influence on the distribution of ions and their adsorptive properties [2].

The interdependency of the particle densities allows to define the influence of electrostatic interactions onto the pressure of solution in porous matrix. The dependence of iones density influence onto solution pressure in pores is calculated.

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Generating functional approach to asymmetric Hubbard model in dynamical mean-field theory

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The generating functional Kadanoff-Baym method generalized to the strongly correlated systems (see [1]) is extended in the present work to the dynamical mean-field theory (DMFT) for such systems. Formulating an approximate analytic scheme for the investigation of the effective single-site problem is our aim. To describe the interaction of a given site with its environment the approach of auxiliary fermions (ξ) is used. The coherent potential is determined as a Green's function of the ξ-field. The generating functional generates by the differentiation the many-particle contributions of a bosonic type to the single-site electron Green's function $G_{i\sigma}(\omega)$. It is taken into account that the expansion around the atomic limit for $G_{i\sigma}(\omega)$ splits into subspaces corresponding to the single-site states $|i,p\rangle$ [2]. This leads to the appearance of the partial irreducible Larkin parts $\Xi_{\sigma}^{(p)}(\omega)$. For $\Xi_{\sigma}^{(p)}(\omega)$ we constructed here functional differential equations.

For the standard and asymmetric Hubbard models in the framework of the iterative procedure a connection with various known approximations is found. It is considered how such a procedure relates with the different-time decoupling scheme in the equations of motion for $G_{i\sigma}(\omega)$ [3], where the GH3 approximation proposed by the authors (a generalization of the Hubbard-III approximation) is revealed to be most successful.

The approximations are tested on some limit cases where it is possible to obtain exact results. Thus, in the Falicov-Kimball limit of the asymmetric Hubbard model, relations between thermodynamic parameters (chemical potentials, particle concentrations) can be found exactly in DMFT. The comparison of the exact thermodynamic results with the GH3 approximation shows that the latter can give reasonable results for high temperatures or large concentrations of localized particles [3].

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Spectral functions of asymmetric Hubbard model in DMFT

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Energy spectrum of the asymmetric Hubbard model is investigated within the dynamical mean-field theory (DMFT). In this model, the chemical potentials and electron transfer parameters depend on the electron spin (type of quasiparticles). The Falicov-Kimball model and the standard Hubbard model can be considered as limit cases of the asymmetric Hubbard model.

Using the projecting technique and different-time decoupling in the equations of motion we construct equations for calculating the mass operator and single-particle Green's functions. The set of equations is obtained in the so-called GH3 approximation that is a generalization of the Hubbard-III approximation [1,2].

In the Falicov-Kimball limit, the approach is used to calculate the spectral function of localized particles for infinite on-site repulsion U and various chemical potentials and temperatures. The comparison of the exact thermodynamic results with the GH3 approximation shows that the latter can give reasonable results for high temperatures or large concentrations of localized particles [2]. The spectrum is broadened by interaction with mobile particles and its form continuously changes from a delta peak to the characteristic form of the density of states of the lower subband in the Hubbard-III approximation when the chemical potential of itinerant particles increases [3].

In the case of the finite U, the Hubbard-I and alloy-analogy approximations are the simplest approximations which are used. Within the alloy-analogy approximation, the energy band of particles does not depend on the transfer parameter of particles of another sort. The GH3 approximation is used in investigating a band structure of the asymmetric Hubbard model at half-filling. A continuous Mott transition with the U_c value dependent on a ratio of transfer parameters of particles of different types is described.

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Theory of dielectric, piezoelectric, elastic and thermal properties of Rochelle salt under a transverse electric field

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A problem of the full description of dielectric, piezoelectric, elastic and thermal properties of the Rochelle salt crystal cannot be solved on the basis of the widely used Mitsui model which is "one-dimensional" by its nature. For such a purpose a four-sublattice pseudospin model allowing to consider an influence of the external transverse electric field $\vec{E} \perp X$ was proposed [1]. We develop here a generalization of this model taking into account the piezoelectric interaction in the crystal [2]. The specific heat, dielectric permittivity components, elastic constants and piezoelectric moduli are calculated. Their anomalies in the phase transition points at non-zero transverse fields $E_2 \parallel Y$ and $E_3 \parallel Z$ are investigated. In particular, the transverse components $\varepsilon_{22}^{\sigma}$, $\varepsilon_{33}^{\sigma}$ have jump-like anomalies in the critical points (with magnitudes of jumps proportional to E_2^2 or E_3^2). Under a field, the temperature region of the ferroelectric phase narrows or broadens depending on the direction of the transverse field. A satisfactory description of the available experimental data is achieved by a proper fit of theory parameters.

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High-frequency cyclotron modes in a Fermi liquid of Q2D layered conductors

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We have studied theoretically the propagation of electromagnetic waves in a Fermi liquid of charge carriers in Q2D layered conductors placed in a strong magnetic field $\mathbf{H}_0$, when the cyclotron frequency of electrons ω_c exceeds significantly the frequency of their collisions. The specific of the Q2D charge carriers energy spectrum in layered conductors results in the oscillatory dependence of the electron drift velocity $\mathbf{v}_H$ along $\mathbf{H}_0$ upon the angle θ between the magnetic field vector and the normal to the layers. For the entire series of the values $\theta = \theta_c$ the velocity $\mathbf{v}_H$ is vanishingly small everywhere at the Fermi surface. This is the case when the collisionless absorption of the wave energy by electrons is absent. At $\theta = \theta_c$ propagation of weakly damping modes with the frequencies close to the cyclotron resonance frequencies $n\omega_c$ (n is an integer) is possible not only for the case when the wave vector $\mathbf{k}$ is normal to $\mathbf{H}_0$, but for an orbitrary orientation of $\mathbf{k}$. We have analyzed the spectrum of the cyclotron modes with regard to the Fermi-liquid interaction between electrons.

Dynamics of charge transfer in quasi-one-dimensional structures with hydrogen bonds

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The model for the description of the charge transfer in quasi-one-dimensional structures with hydrogen bonds is proposed. The model includes the proton-electron interaction which indicate the changes of charges of ions that form hydrogen bond, caused by proton shift on bond, as well as the cooperative proton-electron transport. Band electron spectrum is calculated in the mean field approximation (MFA); the dependence of the mean number of electrons on site on the value of chemical potential μ is obtained. The proton tunnelling frequency, renormalized by the interaction of proton with electron subsystem is calculated. It is established, that system with hydrogen bonds can be in three regimes with different width of electron band and essentially different values of the effective proton tunnelling frequency Ω^{eff}. The frequency dependence of the real part of conductivity is obtained. The possibility of the phase transitions like transformation between uniform phases with different electron concentration n is established depending on the value of chemical potential μ. The phase separation on phases with different width of electron band, different n and Ω^{eff}, and different electron conductivity at the given average electron concentration is obtained.

1.5-multiplicity molecular light scattering in fluids?

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The possibility of experimental registration of the molecular light scattering effects caused by the third thermodynamic moment of the density (ρ) fluctuations has been considered. For this purpose, the contributions from compact groups of scattering centers to the integral intensity of the polarized single scattering in simple fluids are analyzed. After the short-range peculiarities of the electromagnetic field propagator are studied in terms of the theory of generalized functions, the above contributions are separated out from each step of the iteration procedure for the scattered field. In the immediate vicinity of the critical point, the expression for the intensity transforms to the result of the algebra of fluctuating quantities for systems with a conserved order parameter, all the coefficients in the expansion being explicitly restored. In the hydrodynamics region, the individual terms of the series for the intensity are expressed in terms of the second and higher-order thermodynamic moments of the density fluctuations. The analysis with the use of the grand canonical ensemble and the van der Waals equation reveals that the contribution to the permittivity (ε) fluctuations from the third moment of the density fluctuations may exceed that from the Gaussian part of the forth moment. As a result, the former may be detected in the form of the so-called 1.5-scattering of light. This scattering is expected to affect the depolarization ratio Δ of the scattered light. The registration of the effect is most favorable in the case of simple fluids with low values of $(\rho\partial\varepsilon/\partial\rho)$ (such as xenon), when Δ is studied for the temperature interval $10^{-3} \leq \tau \leq 10^{-2}$, $\tau = |T - T_c|/T_c$, and comparable values of $\rho/\rho_c - 1$ near the critical isochore. The experimental data available seem to confirm these predictions.

Adsorption of polymers on the surface with long-range correlated disorder

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Investigation of the influence of long-range correlated surface disorder on the adsorption of long-flexible polymer chains on the wall by applying the field theoretic renormalization group approach directly in $d = 3$ dimensions up to two-loop order was performed. The whole set of surface critical exponents at the adsorption threshold was computed by means of Padé and Padé-Borel resummation techniques. The obtained results indicate that the systems with long-range correlated quenched surface disorder are characterized by the new set of surface critical exponents.

Thermal fluctuations of director orientation in nematic liquid crystals with inclusions

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It is known that in liquid crystals director orientation can be changed easy by external influences and susceptibility of this system is extremely high. This is especially important when investigating system at the close vicinity of phase transition. In this case we have to take into account presence of external fields, interaction with restricting surfaces and presence of impurities as well. Here we consider peculiarities of correlation of director orientational fluctuations in filled system, i.e. system with impurities. Namely we consider different ways of interaction between nematic texture and impurity particles: by means of anchoring interaction of the director with surfaces of impurity particles (for macroscopic particles) and by means of effective interaction energy (for microscopic particles). We show that presence of impurities can cause significant changes in correlative behavior of the system.

Model of the strongly non-ideal electron liquid within the frames of the renormalization interactions theories

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In this paper the structure of the diagrams of the perturbation theory for the electron liquid model in two approaches based on the previous renormalization of the interactions [1, 2] is investigated. In paper [1] renormalization by the method of cyclic transformation of the partition function is realized. In the second approach [2] the rigorous transition from the description in the terms of the secondary quantization operators to the description of the electrons and plasmons in the expanded space of the variables is made. Free electrons with the renormalized energies and free plasmons are the model of the zero approximation. S-matrix is determined by weak interactions (short-range two-electrons, electron-plasmon) and plasmons anharmonicity. Transition operator regulates betweenness relation of the secondary quantization operators of electrons and plasmons.

The principal moment of both approaches is the calculation of n-particles dinamic correlation functions (connected averages)

$$\mu_n(x_1,\ldots,x_n) = \beta^{-1}\left\langle T\left\{\hat{R}_{x_1}\ldots\hat{R}_{x_n}\right\}\right\rangle_0^c \qquad (1)$$

where $\hat{R}_x = \hat{f}_{\mathbf{q},\nu} = \sum_{\mathbf{k},s}\sum_{\nu^*}\frac{\hbar^2}{2m}(\mathbf{k},\mathbf{q})a^+_{\mathbf{k}+\mathbf{q},s}(\nu^*+\nu)a_{\mathbf{k},s}(\nu^*)$ or $\hat{R}_x = \rho_{\mathbf{q},\nu} = \sum_{\mathbf{k},s}\sum_{\nu^*}a^+_{\mathbf{k}+\mathbf{q},s}(\nu^*+\nu)a_{\mathbf{k},s}(\nu^*)$. Functions (1) at $n = 2, 3, 4$ in the analytical form are calculated.

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2. Vavrukh M. V., Slobodyan S. B. // Conden. Matt. Phys., 2005, vol. **8**, p. 472–491.

Calculations of the continuous absorbtion coefficient by the H^- ions in the stellar atmosphere

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The process of photoionization of H^- ion which is the principle mechanism of the stellar photospheres of the Solar-type is described within the frames of the two-electron problem. H^- ion wave function is presented in the form of the expansion of the orthogonal two-electron functions

$$\Psi_{ion}(\mathbf{r}_1,\mathbf{r}_2) \;=\; \sum_{l=0}^{\infty}\Gamma_l\; R_l(r_1,r_2)\; P_l(\cos\gamma),$$

where $P_l(...)$ are the Legandre polinoms, γ is the angle between $\mathbf{r}_1, \mathbf{r}_2$ vectors, and $R_l(...)$ are the symmetric variational functions which account for the radial electron correlations. The expantion coeficients are found from the secular problem, and the parameters of functions $R_l(...)$ derives from the minimization energy pocedure. The final state wave function is constructed in the form of the symmetrical combination for hydrogen atom $1s$ wave function and a free-electron-like one in the hydrogen atomic field.

The momentum operator matrix elements and oscilator strength for the photoionization process have been calculated. The testing of the mentioned phenomenon by the oscilator strength sum rule has proved to be highly accurate (the deviation is not more than 0.5%).

H^- ions dependence on the chemical abundance and photosphere temperature has been stated. The absorbtion coefficient, both in the frequency scale and in the wave-length one, has been researched. The obtained results correspond to the observed data for the Sun.

All the calculations have been made in the analytical form.

The study of the $J_1 - J_2$ s=$\frac{1}{2}$ XXZ chain using the Jordan-Wigner and mean-field approaches

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We study the $J_1 - J_2$ spin-$\frac{1}{2}$ XXZ chain in a spinless fermion representation using the Jordan-Wigner transformation. The ground state properties of the model are studied within a mean-field approach preserving all fermion pair correlations. We determine several mean-field solutions including those which describe dimer phases. Near the limit of the Majumdar-Ghosh model the results of the mean-field approximation are very close to those of an additional complementary analysis of the model which we perform by exact diagonalization. We also obtain the infinite-order phase transition to the dimer state within the approach.

Modificated CPA treatment of one dimensional fermionic models with short range interactions

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Fermionic lattice gas models are suitable for description of ionic and protonic conductors. The simplest example is the well-known spinless fermion model that includes nearest-neighbour interactions as well as the transfer between nearest sites. This model can be used to describe the behaviour of ionic subsystem in objects like superionic crystals. The other fermionic lattice gas model is the so called orientational tunnelling model which is used to describe proton subsystem in various systems with proton conductivity. It takes into account the proton transfer in the spirit of two-stage Grotthuss mechanism and interactions between nearest protons and therefore can be treated as the two-sublattice spinless fermion model.

Short range interactions between ions (protons) are very important and can considerably affect the system's behaviour causing the splitting in ionic (protonic) spectrum. Recently we developed an approach [1] based on the generalization of Week's theorem which allows short-range interactions to be taken into account exactly in the zero-order Hamiltonian. Here we propose another approach based on the the well-known coherent potential approximation (CPA) modified to include short-range interactions into consideration.

Within this approach we study both spinless fermion model and orientational-tunnelling model in one dimensional case. We discuss the spectra of both models at different concentrations of moving particles. We show that in the case of strong short-range interactions both models possess the spectra that are splat into several energy bands. In this case the ionic (protonic) subsystem can be in either quasi-metallic or insulating state depending on average concentration.

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Щорічна конференція в Україні
“Статистична фізика: сучасні проблеми і нові застосування”

Львів, 28–30 серпня 2005 р.

Програма і тези доповідей

Комп’ютерне макетування: Андрій Швайка

Укладання: Олеся Мриглод і Йосип Гуменюк

Формат 84×108/32. Ум. друк. арк. 10,4.
Друк офсетний. Тираж 200 прим.

Друк: ТзОВ “Ю.М.І.”, 2005