INTAS–UKRAINE Workshop on Condensed Matter Physics
(21.05.1998 - 24.05.1998, Lviv, Ukraine)

Responsible organizer	Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine
Supported by	INTAS, Ministry of Science and Technology of Ukraine
Goals	The Workshop aims in promoting and strengthening existing collaboration between physicists working in the field of condensed matter physics. During the Workshop recent studies performed in the frames of INTAS projects will be reported and discussed with the participation of leading scientists from different countries
Main topics	• soft condensed matter (ionic and molecular liquids, disordered systems, polymers); • plasma physics; • critical phenomena; • solid state physics (ferromagnets, metals and alloys, ferroelectrics, semiconductors, hydrogen bonded systems, high–T_c superconductors)
Local Organizing Committee	R.Folk, Yu.Holovatch, O.L.Ivankiv, I.M.Mryglod, I.A.Protsykevych, I.V.Stasyuk
Home page	http://www.icmp.lviv.ua/icmp/ukr-aus.html

INTAS-UKRAINE WORKSHOP on Condensed Matter Physics

Programme

21.05.1998 – 24.05.1998, Lviv, Ukraine

Thursday, May, 21, 1998

Institute for Condensed Matter Physics,
4 Kozelnyts'ka Str., Conference Hall

9.30 – 9.45	**Opening** I.R.Yukhnovskii, R.Vardapetian, A.P.Shpak

Session Chairman: *O.G. Sytenko*

9.45 – 10.20	**M.F.Holovko,** *Lviv* The multidensity integral equation approach in the theory of ionic and complex liquids
10.20 – 10.55	**K.Heinzinger,** *Mainz* On the hydration of ions
10.55 – 11.30	**I.R.Yukhnovskii, M.V.Tokarchuk,** *Lviv* Physical processes in the fuel containing masses interacting with aqueous solutions in the "Shelter" object
11.30 – 11.50	Coffee Break

Session Chairman: *A.Kosevich*

11.50 – 12.25	**E.Krotscheck, K.Schoerkhuber,** *Linz* Single particle and Fermi liquid properties of ^{3}He–^{4}He mixtures: microscopic approach
12.25 – 13.00	**I.O.Vakarchuk,** *Lviv* On the Bose–Einstein condensation in superfluid He^4
13.00 – 13.35	**J.F.Reading,** *Texas* The role of dynamic correlation in a time developing system
13.40 – 14.30	Lunch

Session Chairman: *Z.O.Gurskii*

14.30 – 15.05 **I.F.Goutych, A.G.Sitenko, A.G.Zagorodny,** *Kyiv*
P.P.J.-M.Schram, *Eindhoven*
Magnetic field fluctuation spectra in a plasma with fluid–like random motions

15.05 – 15.40 **P.P.J.-M.Schram,** *Eindhoven*
Dynamics of colloidal crystals

15.40 – 16.15 **M.Cieplak,** *Warsaw*
Kinetics of protein folding

16.15 – 16.35 Coffee Break

Session Chairman: *P.P.J.-M.Schram*

16.35 – 16.55 **S.Katletz, U.M.Titulaer,** *Linz*
A statistical model for antibody–antigen binding

16.55 – 17.15 **V.M.Tkachuk,** *Lviv*
Quasi–exactly solvable potentials with two known eigenstates

17.15 – 17.35 **A.Shimkevich,** *Obninsk*
Fluctuation theory for non-homogeneous melts

17.35 – 17.55 **I.P.Omelyan, M.V.Tokarchuk,** *Lviv*
Generalized dipolar modes of a Stockmayer fluid

17.55 – 18.15 **O.I.Gerasimov, A.N.Kilyan,** *Odesa*
P.P.J.-M.Schram, *Eindhoven*
Kinetic model of ordered colloidal suspensions

18.20 – 19.00 Dinner

19.00 – 21.00 **Poster Session:**

- Soft condensed matter, plasma physics (P1–P27)
  Chairmen: *K.Heinzinger, A.Zagorodny*
- Critical phenomena (P28–P43)
  Chairmen: *R.Folk, Yu.Vysochanskii*
- Solid state physics (P44–P74)
  Chairmen: *M.Kharchenko, E.Schachinger*

Friday, May, 22, 1998

Institute for Condensed Matter Physics,
1 Svientsitskii Str., Conference Hall

Session Chairman: *I.R.Yukhnovskii*

9.30 – 10.05 **H.W.Diehl,** *Essen*
Critical behaviour at interfaces

10.05 – 10.40 **C. von Ferber,** *Tel Aviv*
Collapse of polyampholytes

10.40 – 11.15 **M.P.Kozlovskii, I.R.Yukhnovskii,** *Lviv*
Microscopic approach for description of the critical behaviour of 3D systems

11.15 – 11.35 Coffee Break

Session Chairman: *J.F.Reading*

11.35 – 12.10 **R.Folk, G.Moser,** *Linz*
Critical sound in fluids and mixtures

12.10 – 12.45 **Yu.Vysochanskii,** *Uzhgorod*
Critical behaviour and relaxation effects at the phase transitions in ferroelectrics with semiconductor and ionic conductivity

12.45 – 13.20 **T.Dietl,** *Warsaw*
Ferromagnetic transition in diluted magnetic semiconductors

13.25 – 14.25 Lunch

Session Chairman: *U.M.Titulaer*

14.30 – 15.05 **A.Kosevich,** *Kharkiv*
Soliton complex dynamics in nonlinear dispersive media

15.05 – 15.40 **O.V.Bystrenko, A.G.Zagorodny,** *Kyiv*
Critical phenomena in strongly coupled plasmas and dusty crystal formation

15.40 – 16.05 **I.V.Baryakhtar,** *Kharkiv*
Kinetic equations for solitons in Sine–Gordon and nonlinear Schrödinger equations

16.05 – 16.35 Coffee Break

Session Chairman: *H.W.Diehl*

16.35 – 16.55 **F.Schinagl, R.Folk, H.Iro,** *Linz*
Multicritical behaviour in magnetic fluids

16.55 – 17.15 **I.M.Mryglod, S.Dubyk, Yu.K.Rudavskii,** *Lviv*
R.Folk, *Linz*
Hydrodynamic time correlation functions of a Heisenberg model ferrofluid

17.15 – 17.35 **C. von Ferber,** *Tel Aviv*
Yu.Holovatch, *Lviv*
Scaling exponents for copolymer networks and stars

17.35 – 17.55 **M.Shpot,** *Lviv*
A.Drewitz, *Essen*
Real–space propagator and layer susceptibility at the extraordinary transition

17.55 – 18.15 **O.Myshchyshyn, B.Andriyevsky,**
M.O.Romaniuk, *Lviv*
Critical indices of the ferroelectric phase transition in TGS crystals

19.15 – 21.30 Get–together party

Saturday, May, 23, 1998

Institute for Condensed Matter Physics,
1 Svientsitskii Str., Conference Hall

Session Chairman: *V.Litovchenko*

9.30 – 10.05 **I.V.Stasyuk,** *Lviv*
Local anharmonic effects in high–T_c superconductors

10.05 – 10.40 **E.Schachinger,** *Graz*
Optical conductivity in superconductors with mixed symmetry order parameter

10.40 – 11.15 **E.A.Pashitskii,** *Kyiv*
Charge density fluctuations and gap symmetry in high–T_c superconductors with extended saddle–point features in the electron spectrum

11.15 – 11.35 Coffee Break

Session Chairman: *S.Ryabchenko*

11.35 – 12.10 **M.S.Brodyn, S.G.Shevel, V.V.Tyshchenko,** *Kyiv*
Experimental studies of the dynamics of excitons in II–VI semiconductors (bulk crystals and epilayers)

12.10 – 12.45 **M.F.Kharchenko,** *Kharkiv*
Magnetic field induced structural transformations in the paramagnetic Jahn–Teller crystals of the double alkali rare–earth molybdates

12.45 – 13.20 **V.G.Litovchenko, A.A.Efremov,** *Kyiv*
The enhanced catalytic dissociation of adsorbed hydrogen containing molecules

13.25 – 14.25 Lunch

Session Chairman: *T.Dietl*

14.25 – 15.00 **S.M.Ryabchenko,** *Kyiv*
Magnetooptical investigation of quantum–dimensional structures on the basis of semimagnetic semiconductors

15.00 – 15.35 **M.V.Tkach,** *Chernivtsi*
Quasiparticles in complicated quantum well of nanosizes

15.35 – 15.55 Coffee Break

Session Chairman: *I.V.Stasyuk*

15.55 – 16.15 **R.R.Levitskii, R.O.Sokolovskii,** *Lviv*
Relaxation dynamics of disordered Ising–like models

16.15 – 16.35 **I.V.Brovchenko,** *Kyiv*
Doped molecular crystals as erasable optical information storage

16.35 – 16.55 **V.T.Shvets,** *Odesa*
Hall effect in disordered transition metals

16.55 – 17.15 **Z.O.Gurskii,** *Lviv*
J.Krawczyk, *Opole*
How does one extract many–body interatomic potentials from ab–initio band structure calculations?

17.15 – 17.40 **Closing Session**

Lectures

The multidensity integral equation approach in the theory of ionic and complex liquids

M.F. Holovko

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Recent progress in the integral equation theory of ionic and complex liquids will be reviewed. Particular emphasis is focused on a recent development of the multidensity integral equation approach and its application to the statistical mechanical modelling of a different type of association and clusterisation in liquids. The effects of dimerization, polymerization, solvation, formation of the network bonds and formation of self–assembling systems will be discussed. New application of the integral equation approach for the treatment of the percolation phenomena, the adsorption of fluids in porous media and the description of electronic structure of associative fluids will be illustrated.

The multidensity integral equation approach will be used for the description of adsorption of polymers and network forming fluids on the attractive surfaces. It is demonstrated that cooperative adsorption of the polymeric systems can take place under the conditions of strongly diluted case. This effect recently is verified by the contact–angle measurements of the polymer adsorption. For the network forming systems new type of the cooperative adsorption is discovered which is related to a bridging due to tree–like clusters adsorption. The connectivity properties of the interface are studied and an interfacial percolation threshold is predicted to exist.

Finally the effects of cation hydrolysis and polynuclear ion formation in aqueous solutions of metal salts will be discussed (project INTAS–UA95–133). The theory predicts a significant influence of the polynuclear ion formation on the properties of electrolyte solutions in a wide range of concentrations including very dilute ecological important concentration region.

On the hydration of ions

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The report will concentrate on ions which are produced in nuclear power reactors and/or which are of special interest because of their small radius and/or their high charges. Mainly the results of Molecular Dynamics (MD) simulations will be discussed as they are able to provide a comprehensive and consistent description of the structural and dynamical properties of the water molecules in the hydration shells of the ions. Decisive for the reliability of the results derived from these simulations are the potentials employed. The fact is stressed that they can be tested only by comparison with experimental data which have been derived unambiguously from measurements.

In almost all simulations of alkali halide solutions the ion-water interactions can be described sufficiently accurately by pair potentials. In other cases, like e.g. Be^{+2} or Al^{+3}, three–body interactions have to to be included in the potentials. The effect of the three–body contributions on the structural and dynamical properties of the hydration shell water molecules will be discussed. Whenever reactions between the ions and the water molecules can occur, it will be necessary to employ ab initio simulations such as the Car–Parinello method.

The structural properties of the solutions are discussed on the basis of various radial distribution functions, the orientations of the water molecules and their geometrical arrangement in the hydration shells of the ions. Dynamical properties of the solutions — like self–diffusion coefficients, spectral densities of the hindered translations, librations, and internal vibrations — are derived from the simulations with the help of various autocorrelation functions. They are calculated separately for the three water subsystems — bulk water, hydration water of the cation and the anion. Finally, the effect of metal surfaces on the hydration of ions are mentioned shortly.

Physical processes in the fuel containing masses interacting with aqueous solutions in the “Shelter” object

I.R. Yukhnovskii and M. Tokarchuk

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The main forms of nuclear fuel remaining inside the “Shelter” object and the main interrelated factors of nuclear and ecological danger are considered. Processes of interaction of fuel containing masses with water are analysed on the basis of experimental data. A statistical model for the description of radioactive elements is proposed. The pair structure distribution functions for ions UO_2^{2+}, Cs^+ and Sr^{2+} in aqueous solutions use this model. Chemical reactions of complex formations with the participation of UO_2^{2+} and PuO_2^{2+} as well as reactions of radiolysis in aqueous solutions of radioactive elements are analysed. Nonuniform equations for the description of UO_2^{2+}, Cs^+ and Sr^{2+} ions diffusion from glassy-like fuel containing masses into water and equations of chemical kinetics of radiolysis processes are obtained as well. The shear viscosity and mutual diffusion coefficients of ions UO_2^{2+}, PuO_2^{2+}, Cs^+ and Sr^{2+} in aqueous solutions are calculated numerically for concentrations which are typical of the “Shelter” object.

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Single particle and Fermi liquid properties of ^{3}He–^{4}He mixtures: microscopic approach

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Abstract was not available at printing time.

On the Bose–Einstein condensation in superfluid He^4

I.O. Vakarchuk

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Abstract was not available at printing time.

The role of dynamic correlation in a time developing system

J.F. Reading

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The Response Theorem states that when a quantum eigenstate is perturbed by an external probe it responds initially as if the individual particles were free of all forces, including the interparticle interaction, V_{ij}. Thus for a short time the system can be accurately described by the time development of any convenient independent particle model. By chopping the actual interaction time into segments one can force this impulsive approximation to be accurate: the forced impulse method, FIM[1]. At the end of each segment the system collapses onto a fully correlated set of eigenstates. The length of the segments at convergence contains information about the role of V_{ij}. In a first example of the use of this method we have studied the interaction of fast ions with the correlated electrons in a helium atom[2]. We report the discovery of a new action called pliability which appears to be a characteristic of the helium atom describing the fluidity of the electrons under the influence of the projectile probe. The pliability decreases linearly as the charge of the projectile increases from negative to positive, indicating that the induced change in the density of electrons increases the role of V_{ij}.

1. Reading J F, Ford A L, Smith J S and Becker R L 1984 in *Electronic and Atomic Collisions* edited by Eichler J, Hertel L V and Stolterfoht N, Elsevier, New York, 201-11

2. Reading J F, Bronk T and Ford A L, 1997 a) J. Phys.Rev.Lett.78 749; b) J.Phys.B.30 L189-95; c) Nucl.Instr.Meth. B 132 231-235.

Magnetic field fluctuation spectra in a plasma with fluid-like random motions

I.F. Goutych[a], A.G. Sitenko[a], A.G. Zagorodny[a], and P.P.J.-M. Schram[b]

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The theory of electromagnetic fluctuations in stable stationary plasmas is generalized to the case of plasmas with fluid-like random motions (turbulent plasmas). To provide such generalization the kinetic equation of the Fokker-Planck type is introduced to take into account the influence of large-scale random perturbations on microscopic fluctuations. The probability of particle transitions in the phase space (Green's function) is calculated with regard for turbulent perturbation influence on plasma particle motion.

Dielectric permittivity tensor and correlation functions of the Langevin sources for turbulent plasma are found and general relations for electromagnetic field fluctuation spectra are derived.

Detailed numerical analysis of magnetic field fluctuation spectra distributions is carried out and peculiarities of spectra associated with collective fluctuations in magnetoactive plasmas are found. In particular, it is shown that magnetic field fluctuation spectra in the low-frequency domain (at frequencies much less than ionic cyclotron frequency) have incoherent part (near zero frequency) and collective maxima due to Alfen and magnetosound wave excitation. The influence of thermal effects on collective fluctuations is studied in detail.

Dynamics of colloidal crystals

P.P.J.-M. Schram

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The dynamic behaviour of colloidal crystals is characterized by excitation of waves due to Brownian motion and strong damping by fluid friction. Colloidal systems with 3 components (macroions, counterions and electrons) and large charge asymmetry are considered. Both kinetic and visco-elastic theory are used for the derivation of dispersion relations for longitudinal and transverse modes. The visco-elastic approximation is valid in the case of long wavelengths. In literature there is some confusion about the influences of counterionic diffusion, other plasma phenomena and finite crystal sizes. In our theory these effects are all consistently taken into account. The finite size effects are very pronounced. The results are compared with recent experiments in our own group and the (considerable) discrepancies between theoretical and experimental results are discussed.

Kinetics of protein folding

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Functionally useful proteins are sequences of aminoacids that fold rapidly under appropriate conditions into their native states. It is believed that the phase space of conformations for rapid folders has the structure of a folding funnel. While there are many experimentally accessible predictions pertaining to the existence of such funnels there have been relatively few studies in the controlled setting of well-characterized lattice models. The authors work on the kinetics of folding in the lattice models of proteins explores comparisons to glasses and spin glasses. In particular, by using the steepest descent landscape mapping techniques of Stillinger and Weber, employed originally in the context of supercooled liquids, one may provide an operational definition of the folding funnel and study its properties. The funnel is identified through a coarse grained mapping of the states of the system into maximally compact conformations and obtaining significant connectivities between them. In order to identify kinetic traps in the folding process, an exact master equation approach to folding in a 12 monomer sequence is used. A structure-based design of sequences which have a target structure as the native state along with thermodynamic stability and kinetic accessibility is proposed.

1. Lattice model for rapidly folding protein-like heteropolymers, I. Shrivastava, S. Vishveshwara, M. Cieplak, A. Maritan, and J. Banavar, Proc. Natl. Acad. Sci. 92, 9206 (1995)
2. Cell dynamics of model proteins, M. Cieplak, S. Vishveshwara, and J. R. Banavar, Phys. Rev. Lett. 77, 3681 (1996)
3. Cell dynamics of model proteins, M. Cieplak and J. R. Banavar, Folding and Design 2, 235 (1997)
4. Structure-based design of model proteins, J. R. Banavar, M. Cieplak, A. Maritan, G. Nadig, F. Seno, and S. Vishveshwara, Protein: Structrure, Function and Genetics (in press)
5. M. Cieplak, M. Henkel, J. Karbowski, and J. R. Banavar, Master equation approach to protein folding and kinetic traps (in final preparation for Phys. Rev. Lett.)

Critical behaviour at interfaces

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A survey of recent results on critical behaviour at interfaces is given, with emphasis on the surface critical behaviour at continuous disorder-order transitions of bcc binary alloys such as FeCo. For such systems the universality class describing the surface critical behaviour depends in general on the orientation of the surface plane with respect to the crystal axes [1,2].

1. A. Drewitz, R. Leidl, T. W. Burkhardt, and H. W. Diehl, Phys. Rev. Lett. **78**, 1090 (1997).
2. R. Leidl and H. W. Diehl, Phys. Rev. A **57**, 1908 (1998).

Collapse of polyampholytes

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The main motivation for studying the conformations of randomly charged polymers (polyampholytes - PA) is the interest in understanding protein folding. Due to the long-range electrostatic interactions the low temperature conformations of a PA are very sensitive to its total excess charge Q. While randomly charged PA's with $Q = 0$ collapse at low temperature T, the size of PA's above a critical charge $Q > Q_c$ increases for low T. The PA finds the following preferred configurations: Segments of the chain, which have an overall vanishing charge collapse to globules, while highly charged segments stretch out in between. Monte Carlo (MC) simulation and exact enumeration [2] support this 'necklace' picture of a typical PA configuration. An important question concerns the size distribution of the globules along the chain, especially the distribution of the largest globule. More generally the answer is given by the distribution of the largest segment of charge Q found on a randomly charged chain. This distribution has been determined by MC simulations [3]. It appears to attain a universal shape for long chains while displaying an unexpectedly rich structure.

Here we approach the problem by a self-avoiding walk model with a specially adapted interaction. The zero charge segments of the chain are modelled as loops in a random walk. We exclude all configurations with loops larger than a given L. The conformation statistics of this model, yields the size distribution of the largest Q segments. We have calculated the perturbation theory for this model. In the small coupling limit the results compare well to corresponding MC simulations, which have been performed recently It may be shown that the interaction introduced here renormalizes in the same way as the interaction between mutually avoiding walks studied earlier [4]. Apparent singularities in the distribution of neutral segments are explained and their respective asymptotic behaviour is calculated by renormalization group methods.

1. Y.Kantor, H.Li, and M.Kardar. PRL 69:61, 1992. PRE 49:1383, 1994.
2. Y.Kantor and M.Kardar. PRE 52:835, 1995.
3. L.Schäfer, U.Lehr, and C.Kappeler. J Phys. I, 1:211, 1991.
4. D.Ertas, Y.Kantor PRE 53:846, 1996; C. von Ferber, Y.Holovatch EPL 39:31, 1997.

Microscopic approach for description of the critical behaviour of 3D systems

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Analytical method for the description at a phase transition in a three–dimensional spin system is suggested. The method is based on the use of non-Gaussian distribution for fluctuations of spin moment densities and enables to represent the critical behaviour near a phase functions of an Ising–like system with exponentially decreasing interparticle potential are obtained. Their dependence on the temperature is researched as well as that on microscopic parameters of a model (lattice constant, parameters of an interaction potential).

Critical sound in fluids and mixtures

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The behaviour of sound is explained within the dynamical renormalization group theory. Non asymptotic effects are due to the deviation of renormalized couplings from their fixed point values. We calculate the temperature and frequency dependence of the sound velocity and absorption near the consolute point and the gas liquid critical point in pure fluids and mixtures. The critical non asymptotic time scale in mixtures is different from the pure fluid case and set by an effective order parameter Onsager coefficient containing the dynamical parameter related to the enhancement of the thermal conductivity. We discuss the relation to the phenomenological theory of Ferrell and Bhattacharjee for the consolute point and compare with experiments in ^{3}He-^{4}He mixtures near the plait point. For pure fluids we present the comparison with Xe, CO_2, and He.

This work is supported by the Fonds zur Förderung der wissenschaftlichen Forschung (Project 12422-TPH)

Critical behaviour and relaxation effects at the phase transitions in ferroelectrics with semiconductor and ionic conductivity

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The crystals of complex chalcogenides $M'M''P_2S(Se)_6$ with a three-dimensional lattice or with layered structure and with cations in different charge state have different types of dipole ordering in presence of semiconductor or ionic conductivity.

For the crystals like $Sn_2P_2S(Se)_6$ with a three- dimensional lattice mainly displacive phase transitions occur but also order-disorder effects are observed. Here on the inelastic neutron scattering and Raman spectroscopy data the interaction between the soft optic mode and acoustic phonons is at the origin of the incommensurate phase formation. The fluctuation effects appearance near the phase transitions temperatures is in agreement with conclusions of the renormalization-group theory for the Lifshitz point in proper uniaxial ferroelectrics with one direction of modulation at taking into account its closeness to tricritical point on the state diagram. For these ferroelectrics-semiconductors the relaxation of an electron subsystem determines the Lifshitz point shift on the phase diagram and the pinning of the order parameter wave (memory effect) in the incommensurate phase. The freezing of the relaxation dynamics of the incommensurate modulation is observed at low temperatures. The amorphous dielectric behaviour of the incommensurate phase in region 0,01 - 7K is described in the two-level system model.

The layered crystals $CuInP_2S_6$, $CuCrP_2S_6$ undergo order- disorder type transitions to ferroelectric or antiferroelectric phases. Here the critical relaxation dynamics of Cu+ ions is connected with the thermal “throw” of Cu+ ions into interlayer space and also with the ionic conductivity.

Ferromagnetic transition in diluted magnetic semiconductors

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It has been known for a long time that the compensation of antiferromagnetic interactions between the localized spins by a ferromagnetic coupling would result in a dramatic enhancement of the sensitivity of diluted magnetic semiconductors (DMS) to temperature and magnetic field. Search for the ferromagnetic transition has so far been successful in the case of Mn-based IV-VI [1] and III-V compounds [2].

Recent progress in epitaxial doping of II-VI wide gap semiconductors by *substitutional* impurities has stimulated a detail analysis of the nature and strength of the carrier-mediated spin-spin interactions in bulk, layered, and nanostructured II-VI compounds [3]. It has been found that the p-type doping may constitute an efficient tool to enlarge the magnetic effects in wide gap II-VI DMS and their quantum structures.

Indeed, the presence of a ferromagnetic transition in single, modulation-doped, 8 nm quantum well of $Cd_{1-x}Mn_xTe/Cd_{1-y-z}Mg_yZn_zTe$:N is put into the evidence by observing colossal Zeeman splittings of interband optical transitions, probed by means of photoluminescence and its excitation spectra [4]. The transition occurs at 1.8 K for $x = 0.024$, and is driven by long range Ruderman-Kittel-Kasuya-Yosida interactions between Mn spins, mediated by 2×10^{11} holes per cm^2. A quantitative description of the findings confirms predictions of the model [3] on the free carrier-induced ferromagnetism in structures of doped DMS. It makes also possible to evaluate the strength of many body effects for the case of two-dimensional hole gas. At the same time, the data provide important information on critical phenomena in the disordered magnetic systems of reduced dimensionality illustrating, in particular, how long range spin-spin interactions stabilize an ordered phase and make fluctuations of magnetization irrelevant.

1. P. Łazarczyk, T. Story, M. Arciszewska, and R.R. Gałązka, *J. Magn. Magn. Materials* **169** (1997) 151, and reference therein.
2. See, S. Koshihara *et al.*, *Phys. Rev. Lett.* **78** (1997) 4617; Jing Shi, S. Gider, K. Babcock, and D.D. Awschalom, Science **271**, 937 (1996), and references therein.
3. T. Dietl, A. Haury, and Y. Merle d'Aubigné, *Phys. Rev. B* **55** (1997) R3347.
4. A. Haury, A. Wasiela, A. Arnoult, J. Cibert, S. Tatarenko, T. Dietl, and Y. Merle d'Aubigné, *Phys. Rev. Lett.* **79** (1997) 511.

Soliton complex dynamics in nonlinear dispersive media

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Dynamical properties of topological solitons in strongly dispersive medium are investigated. It is shown that the solitons possess an internal structure and their interaction depends on intrinsic properties such as the flexibility. As a result identical solitons can attract each other and form the bound soliton complex. The complex can move without any radiation in strongly dispersive media.

It is also shown that this phenomenon belongs to class of the universal dispersive effects which can be realized in both discrete and continuous media. We present a number of physical models bearing the soliton complexes. The models are described by partial differential nonlinear equations with fourth and higher spatial or mixed derivatives. Solutions of the equations can be obtained numerically and analytically. We found exact analytical solutions for several variants of the dispersive sine-Gordon (dSGE) and double sine-Gordon equations (dDSGE).

It is found that soliton complexes can be also realized as a discrete set of solitonic configurations with internal radiation-like structures. We propose the classification of these "excited states" of soliton complexes, constructing them explicitly in the framework of the double piecewise dispersive model. The two soliton ansatz approximation is used to find analytically the existence condition for the soliton complex in the dSGE and dDSGE. We find numerical solutions of these equations for two-soliton complexes and its "excited states" and their dependences of energies, momenta and velocities on the model parameters. As a result we have formulated the concept of the topological soliton complex and developed the theory of the radiationless dynamics of this coherent solitonic structures as a universal effect in strongly dispersive medium.

Critical phenomena in strongly coupled plasmas and dusty crystal formation

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Critical phenomena in strongly coupled plasmas are studied by means of analytical model description and Monte-Carlo simulations.

The effective potentials in many component charged hard sphere mixture are calculated within the model integral equations derived in HNC-approximation. Critical behaviour of such potential which could be interpreted as a spatial ordering tendency is discussed.

Monte-Carlo simulations of strongly coupled Coulombic systems are performed in attempt to describe dusty crystal formation. Dusty plasma is treated as a set of two sorts of hard spheres of the opposite charge interacting with Coulombic forces. Simulations were carried out for NVT-ensemble. Three following types of the model were studied:

i) finite system consisting of several immobile grains in neutralizing background;

ii) infinite system with periodic boundary conditions with various charge asymmetry (ratio of grain charge to background particle charge);

iii) one component system of highly charged hard spheres in neutralizing background.

As a result of simulations critical behaviour of the systems under consideration is studied and critical values of plasma parameters were found. It is shown that the phase transition associated with the plasma particle condensation on grains can be observed. The lattice formation is predicted for high charge asymmetry (grain charge number greater than 30).

Local anharmonic effects in high–T_c superconductors

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Interaction of electrons with locally anharmonic lattice modes is the one of possible mechanisms of the increasing of the effective electron attraction constant and raising of the transition temperature into superconducting state. In high–T_c superconductors with $YBa_2Cu_3O_{7-\delta}$ structure the sublattice of apex oxygen O_4 ions plays the role of the subsystem for which the local anharmonicity is the characteristic feature. The evidence of that is the existence of two equilibrium positions for O_4 ions. Their occupancy changes with temperature and oxygen stoichiometry δ. The influence of local anharmonicity on the electron spectrum and thermodynamics of the system is studied mainly in the framework of pseudospin–electron model, where the O_4 ion motion is described by pseudospin formalism and electron correlation is taken into account in the spirit of Hubbard model.

We consider in this lecture a number of effects occurs in this model:

- phase transitions connected with the reorientation of pseudospins;
- ferroelectric type instabilities and conditions of the noncentrosymmetric phases appearance;
- possibility of formation of the charge ordered states with spatial modulation;
- phase separation effects in pseudospin as well as electron subsystems;
- bistability phenomena in pseudospin sublattice under the influence of oxygen vacancies random field;
- peculiar behaviour of the transverse dielectric susceptibility and charge–charge correlation function in the regions of the above mentioned instabilities.

The comparison of the results obtained in the different approximations (including GRPA, static and dynamic (in the limit $d = \infty$) MFA) and for the various model parameters values is given. The experimental manifestation of the effects under consideration is discussed.

Optical conductivity in superconductors with mixed symmetry order parameter

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The large anisotropies observed in the in-plane transport properties of untwined single crystals of $YBa_2Cu_3O_{6.95}$ reside in the orthorhombic nature of its band structure which includes CuO chains as well as CuO_2 planes. An infinite band model with distinct effective mass in a and b-direction is used to study the a.c. conductivity of a d-wave BCS superconductor. A subdominant s-wave admixture is also included in the gap because both symmetries belong to the same irreducible representation in an orthorhombic system. Theoretical predictions are compared to experiment. The pronounced differences in the real and imaginary part of the optical conductivity and the derived scattering rate of superconductors with mixed $s + d$ or $s + id$ symmetry order parameter are discussed for different mixing and for moderate impurity concentrations in the two limiting cases, namely the Born (weak) and the resonant scattering (unitary) limit. Adding unitary impurities to a system with an $s + d$ symmetry order parameter should, in some cases, allow one to determine the amount of a subdominant s-wave component by measuring the frequency dependence of the optical scattering rate.

Charge density fluctuations and gap symmetry in high T_c superconductors with extended saddle-point features in the electron spectrum

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This talk is devoted to the topic of superconducting order parameter symmetry in high-temperature superconductors. Both experimental and theoretical aspects of this problem are considered, with the emphasis on the role of the extended saddle-point features (ESPF) observed in the electronic spectrum of cuprates in the angular resolved photoemission spectroscopy (ARPES) experiments. The ESPF strongly effect the spectrum of the collective electron-density excitations, the screened Coulomb interaction, and also the superconducting gap symmetry. Their existence leads, in particular, to the appearance of a low-frequency peak in the spectral function of the charge density fluctuations due to the presence of acoustic plasmon branch in the collective electron spectrum. The retarded anisotropic electron-plasmon interaction brings about the suppression of the static screened Coulomb repulsion for small transferred momenta and, consequently, the effective attraction between electrons in the $d_{x^2-y^2}$-wave channel of the Cooper pairing of current carriers. Violation of C_{4v} symmetry in *BSCCO* and *YBCO* crystals leads to a possibility of a change of $d_{x^2-y^2}$-wave symmetry of the gap to mixed $s-d$ gap symmetry for singlet Cooper pairs or to p-wave gap symmetry for triplet pairs.

Experimental studies of the dynamics of excitons in II-VI semiconductors (bulk crystals and epilayers): collaborative INTAS project

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The experimental studies of the properties of luminescence have been performed with the aim to get better understanding of the dynamical behaviour of carries (excitons) in II-VI semiconductors. Two classes of objects were under study: first, CdS bulk (platelet) crystals and few μ thick crystalline epilayers and, second, ZnSe quantum wells (of 1.1 nm thickness) with ZnS barriers grown by photo-assisted vapour phase epitaxy.

For CdS bulk crystals and epilayers the effect of the broad-scale variation of an excitation level I_{exc} has been studied not only for excitonic but also for the donor- acceptor pair (DAP) luminescence. In bulk crystals DAP luminescence is found to exhibit more complicated behaviour with the increase of I_{exc} up to damage threshold than the simple saturation commonly assumed earlier without the experimental verification. In contrast, in epilayers such saturation does occur. The qualitative explanation is suggested that takes into account the role of the (non)diffusive transport of carriers (excitons) beyond the active near-surface region under a single-photon excitation.

In the spectra of ZnSe quantum well the evidences of interface disorder are found. The observed dependences of the excitonic luminescence spectra on excitation power and temperature are interpreted by a model involving exciton localization by random potential caused by well thickness fluctuations. The mobility edge is measured for these samples to be 6 meV below the free exciton energy in the ideal quantum well.

Magnetic field induced structural transformations in the paramagnetic Jahn-Teller crystals of the double alkali rare-earth molybdates

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Experimental investigations on the influence of a magnetic field on the lattice structure transformations in the magnetically unordered paramagnetic crystal were undertaken with the layered mica-like crystals of the double alkali rare-earth molybdates that have very strongly anisotropic magnetic Jahn-Teller centres.

The subjects of investigations were the KDy- and KEr- molybdates. As result of carried out investigations the new spontaneous and magnetic field induced intermediate crystalline phase in the KDy-molybdate has been revealed. It has been experimentally found that the intermediate phase can be induced by magnetic field applied along direction over a wide range of angles. Those facts that the low-field transition is accompanied by a hysteresis with its tails penetrating deeply in the intermediate and low-field phases whereas the high-field transition occurs without a hysteresis together with the peculiar behaviour of the linear birefringence in the intermediate temperature region suggest that the intermediate crystalline state is the magnetically sensitive incommensurate modulated phase.

In the KEr-molybdate the microwave field induced regular and chaotic motions of the crystal lattice have been observed in the vicinity of the critical point of the structural instability caused by the external magnetic field applied along the certain direction. The features of the relaxation absorption, which have a threshold character with respect to the microwave power pumping, have been revealed. It has been assumed that observed bifurcations of the microwave absorption are induced by occurrence of the dynamic dissipative structures of the crystal lattice vibrations.

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The enhanced catalytic dissociation of adsorbed hydrogen containing molecules

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The incorporation into the surface of such classical catalysts as Pt or Pd some impurities allows us to variate in large degree its activity as to dissociation of hydrogen containing molecules. The same effect is often observed in the case when the respective impurity atoms are not incorporated but only adsorbed on the surface. Such influence, in general case, may be treated as a modification of a shape of potential curve (the change of the first barrier height, appearance of additional pre-chemisorption states etc.) for interaction between molecule and substrate.

There are several reasons for such transformations. For transition metals it may be, e.g. the reorientation or reattachment of surface chemical bonds, electronic transfer between the substrate atom and the impurity. Another important point is connected with an appearance of the long range Coulomb interaction in the system. Empirical data show that the electropositive (in respect to the Pd substrate) impurities (K, Cu, Fe, Ni) act as the promoters for catalytic reactions. On the other hand electronegative impurities (P, S or O) act as catalytic poisons. The most accepted explanation of this phenomena is the increase (or decrease) of the residence time of the molecule in the pre-chemisorbed state due to electrostatic effects. For hydrogen containing molecules the pre-chemisorbed state is controlled, as a rule, by hydrogen bonding. So, the doping of the surface of the substrate by electropositive atoms or coadsorption of them together with hydrogen containing molecules may give a good tool for study of the role of hydrogen bonding in surface reactions.

We shall present here the experimental data showing the promotion of dissociative adsorption of hydrogen on Pd surface in the present of Cu (case of CuPd surface alloy), or water molecules (the case co-adsorption on Pd surface). The respective calculations for surface reactions kinetics will be made also.

Magnetooptical investigation of quantum-dimensional structures on the basis of semimagnetic semiconductors

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It is proposed the short review of possibilities for obtaining of information about a confinement states of charge carriers, about a interfaces quality and other peculiarities of quantum wells (QW) in semiconductors by using of semimagnetic materials. In particularly, some results of INTAS grant #93-3657 will be discussed.

Semimagnetic (or diluted magnetic) semiconductors are the heteropolar solid solution of semiconductors with substitution of part of cation positions on the isovalence magnetic ions. One of typical representation of it is, for instance, the $Cd_{1-x}Mn_xTe$. In combination with other solid solution of semiconductors it may be used for creation of different heterostructures. The semimagnetic materials are used both for QW and for barriers, or one part of heterostructure components is a usual semiconductor and other is a semimagnetic one.

The main effects in semimagnetic materials are connected with carrier-ions exchange interaction and, in part, with antiferromagnetic exchange interaction between the magnetic ions. In the heterostructures with semimagnetic materials new possibilities for stabilisation of 2D magnetic polarons and for controlling of confinement potential by the external magnetic field arise.

The first of discussed effects is the paramagnetic enhancement of the giant spin splitting (GSS) of confinement excitons in nonmagnetic QW with semimagnetic barriers. As have been established, it is connected with two reasons: i) decreasing of possibilities to form an antiferromagnet spin complexes in nearest to interface monolayers of barrier, and ii) partial intermixing of QW and barrier materials in neighbourhood of interface.

The second of discussed effects is connected with asymmetry of QW in the real growth process. It leads to asymmetry in paramagnetic enhancement of the GSS in systems with different barriers in dependence on growing direction and remove the forbidding of the optical transition between the valence and conducting bands confinement states with different parity quantum number of states.

The information about interface quality, which may be obtained on the base of mentioned effects is discussed.

Quasiparticles in complicated quantum well of nanosizes

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Phase transitions in ferroelectrics

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For the Ginsburg-Devonshir model of ferroelectrics the theory of second order phase transition on the basis of kinetic equation for the distribution function of a relative displacement values for sublattices ("order parameter"), coordinates and time is developed. The account of ferroelectric characteristics is carried out for all values of temperature in the critical region for the one-domain as well as for polydomain states.

The account of the fluctuations of "order parameter" is also carried out. It is shown that the Orstein-Zernike formula is valid not for the space correlator of fluctuations, but only for the spectral density of the space correlator at zero frequency. This explains the observed by the experiment the dependence of the spectral line halfwidth on the correlation radius and the wave number. The smallness of the correlation parameter for all values of temperature serves for the justification of adopted approximations.

Correlation entropy of nonequilibrium quantum gases

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The nonequilibrium thermodynamic entropy is calculated for quantum systems described by the single-particle, f_1, and two-particle, f_2, density matrices. The thermodynamic entropy $S[f_1, f_2]$ is defined as the entropy in the generalized Gibbsian ensemble (the relevant ensemble) in which the single-particle and two-particle density matrices coincide with the true nonequilibrium density matrices. The corresponding consistency conditions may be considered as nonequilibrium equations of state [1].

Using perturbation expansions of the nonequilibrium equations of state, explicit expressions for $S[f_1, f_2]$ are obtained in two limiting cases — for systems of weakly interacting quasiparticles and low-density gases. In both cases, the nonequilibrium entropy can be represented in the form $S[f_1, f_2] = S_0[f_1] + S_{\rm corr}[f_1, g_2]$, where $S_0[f_1]$ is the entropy of an ideal gas, and $S_{\rm corr}[f_1, g_2]$ is the correlation entropy which depends on the two-particle correlation matrix g_2.

The correlation entropy of nonequilibrium low-density gases involve the leading density corrections and contributions associated with bound states of the particles. In the classical limit, the density corrections coincide with the correlation entropy of nonequilibrium classical gases [2].

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Critical behaviour of 2D weakly disordered anisotropic spin systems

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The critical behaviour of two-dimensional (2D) anisotropic systems with weak quenched disorder described by the so-called generalized Ashkin-Teller model (GATM), including the Ising model (IM) with random bonds, the dilute Baxter model, the impure N-colour Ashkin-Teller model, and minimal conformal field theory models (MCFTM) with $c < 1$ (c is the central charge) perturbed by randomness is discussed. It turns out that near criticality the GATM is equivalent to a finite set of Ising planes coupled together through their local energy densities. Using the Grassmann path integral representation for the partition function of the 2D IM and the replica trick the effective action may be rewritten in terms of a 2D multifermion field theory similar to the Gross-Neveu model with a few independent quartic coupling constants [1,2]. All the above models except MCFTM were found to belong to the Ising model universality class. The critical exponents of disordered MCFTM are calculated in the framework of perturbation theory in powers of $\epsilon = c - 1/2$. The numerical values of critical exponents for dilute MCFTM are very close to those of the pure 2D Ising model [2]. This result supports the conjecture (valid only approximately for the MCFTM) of a superuniversality for the 2D disordered models with discrete symmetries. Renormalization group flows exhibit rounding the fluctuation-driven first-order phase transitions by randomness [3].

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A statistical model for antibody-antigen binding

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We discuss a statistical model for antibody-antigen binding. The two macromolecules are assumed to be linked by a number of relatively weak bonds (or groups of correlated bonds) that are assumed to open and close statistically. We use the model to analyze experiments performed in the Institute of Biophysics at the Johannes Kepler University. In these experiments the two molecules are brought into contact using an atomic force microscope; then a prescribed time dependent force is applied to the bond and the distribution of times needed to pull the molecules completely apart is measured. This quantity is calculated with our model; its dependence on the model parameters (binding free energies, number of elementary bonds, force dependence of the binding free energy) is determined.

Quasi-exactly solvable potentials with two known eigenstates

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A new supersymmetry method for the generation of the quasi-exactly solvable (QES) potentials with two known eigenstates is proposed. Using this method we obtained new QES potentials for which we found in explicit form the energy levels and wave functions of the ground state and first excited state.

Fluctuation theory for non-homogeneous melts

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Generalized dipolar modes of a Stockmayer fluid

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Dielectric relaxation in polar fluids was the subject of many investigations in theory, computer simulation and pure experiment. Despite such intensive studies, some key problems still remain unsolved even in the simplest case of a point dipole system. Recently, the concept of generalized collective modes, proposed initially to investigate simple fluids, has been applied to a dipolar system. However, the dielectric quantities have been calculated here with the help of a fitting procedure, because higher-order correlation functions were not known.

In the present study, the generalized dipolar mode spectra of a Stockmayer fluid are evaluated over a wide scale of wavelengths within up to the five-order description without involving any adjustable parameters. In the framework of the proposed approach, the frequency dependence of dielectric quantities is determined by extended continued fractions to which the Markovian approximation is applied. As a result, it is shown that the three-variable theory reproduces qualitatively the wavevector- and frequency-dependent dielectric constant, whereas starting from the five-order description one can talk about the quantitatively reproducing over the whole range of varying wavenumbers and frequencies. Moreover, we demonstrate that within the same approximation all times constants of memory kernels can be expressed in terms of static correlation functions, so that the dynamic properties of the system are described using static fluctuations exclusively. A relationship of the theory proposed with existing approaches is established.

Kinetic model of ordered colloidal suspensions

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Physics of an assembly of spheres has been a subject of intensive interest for a long period of time because of importance of many areas of condensed matter physics. In particular in [1] the critical mode analysis in the case of model colloidal system with the ordering have been carried out on a basis of an integral equation's method from the liquid matter theory. The model of complex multicomponent colloidal systems which consist of charged and neutral hard spheres (which have also a permanent dipole moments) was studied in details. Within the present paper the influence of the internal model parameters on the structural parameters of ordered state is investigated. On an example of water suspension of polystyrene a positive role of the detalisation mentioned v.s. in description of colloidal systems (especially - multicomponent character) with respect to possibility to give a more realistic estimates for the structural parameters of ordered state will be clearly demonstrated. Namely, three-component compound model which includes macroions, counterions and water matrix will be discussed in comparison with a two- and one-component models for such a systems. The better agreement between the theory and experiment is observed in the case of detailed three-component model.

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Kinetic equations for solitons in Sine-Gordon and nonlinear Schrödinger equations

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The investigations of solitons has been started in 1965 when N. J. Zabusky and M.D. Kruskal discovered unusual property of solitary waves: they interact without changing forms and velocities in simple plasma model. It means that there is no thermalization in the system of solitons. Since then, soliton problem is the matter of concern. In the present report kinetic equations have been constructed for different types of localized excitations in Sine-Gordon equation and for envelope solitons in nonlinear Schrödinger equation. Transport equation has been derived from kinetic equation following the standard way and kinetic coefficients have been calculated. The influence of the interactions which destroy the integrability of the model has been considered. It has been shown that the relaxation of soliton gas in the model closed to the integrable has two steps. First step deals with shifts of solitons positions and second one - with momentum exchange. Diffusion coefficient in this case is the sum of two terms. That means that corresponding relaxation processes are increased comparing with the absence of one of the processes. The possibility to apply the proposed theory for kinetic effects analysis in plasma and solids are considered.

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Multicritical behaviour in magnetic fluids

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The phases of a magnetic fluid in an external field are considered. As model systems we take an ideal (hard core) gas with Ising interaction and a van der Waals gas with additional Heisenberg interaction. In mean field approximation various phases and critical points are identified. For appropriate values of the ratio of the magnetic and non-magnetic interactions multicritical points like tricritical points and critical end points exist. For the ideal Ising fluid we calculate the line of wing critical points analytically and prove classical tricritical behaviour. In the van der Waals case wing critical points and the gas-liquid critical point may coexist. The corresponding phase diagrams in (p, t, h)-space are shown.

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Hydrodynamic time correlation functions of a Heisenberg model ferrofluid

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For a Heisenberg model ferrofluid, using the results obtained previously [1], we derived the analytical expressions for all the hydrodynamic time correlation functions (HTCFs) constructed on the set of conserved dynamic variables (the densities of particles number, momentum, energy and magnetic momentum). In the hydrodynamic limit the obtained results are asymptotically exact. The weight coefficients describing the contributions fron each of the hydrodynamic modes are calculated by the perturbation theory taking into account the terms of the second order with respect to a small parameter k, where k is a wavenumber. It is shown, that in case of zero external magnetic field $h = 0$, the HTCFs of a fluid subsystem can be written in the form known for a simple liquid [2] and the "spin-spin" HTCF is given by a single term related to the spin diffusion mode. When h is nonzero an additional coupling between subsystems appear and all the modes contribute to the "density-density" and "spin-spin" HTCFs. An expression for the Landau-Placzek ratio of the integrated intensities of the central Reyleigh line to the shifted Brillouin lines is derived.

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Scaling exponents for copolymer networks and stars

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We explore and calculate the rich scaling behaviour of copolymer networks in solution by renormalization group methods. We establish a field theoretic description in terms of composite operators. Our 3rd order resummation of the spectrum of scaling dimensions brings about remarkable features: The special convexity properties of the spectra allow for a multifractal interpretation while preserving stability of the theory. This behaviour could not be found for power of field operators of usual ϕ^4 field theory. The 2D limit of the mutually avoiding walk star apparently corresponds to results of a conformal Kac series. Such a classification seems not possible for the 2D limit of other copolymer stars. We furthermore provide a consistency check of two complementary renormalization schemes: epsilon expansion and renormalization at fixed dimension, calculating a large collection of independent exponents in both approaches.

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Real-space propagator and layer susceptibility at the extraordinary transition

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The experimentally observed phenomenon of critical adsorption occurring close to the demixing point in liquid binary mixtures confined by a plane hard wall or interface provides a prominent example of the extraordinary phase transition. The important characteristic feature of this transition is that the surface is ordered both above and below the critical temperature and a non-vanishing order-parameter profile is present in both phases. We present a theoretical study of the critical behaviour of the order-parameter correlation function at the extraordinary transition in semi-infinite systems. Using methods of conformal field theory we have obtained the real-space representation for the free mean-field propagator at criticality in arbitrary spatial dimensions $d \leq 4$. We succeeded in revealing a simple algebraic structure of the propagator which provides practical possibility of higher-order calculations. Employing this representation we have calculated the explicit expression for the layer susceptibility at the extraordinary transition in the one-loop approximation. Our result holds for arbitrary width of the layer and its position in the half-space.

Critical indices of the ferroelectric phase transition in TGS crystals

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Temperature dependences of relative changes of geometric thickness $\Delta l/l$ and susceptibility $\Delta\eta/\eta$ of ferroelectric triglycine sulphate crystal (TGS) are investigated in the range of $39\ldots80$°C on the basis of original laser interferometer technique for measuring the temperature induced change of optical path differences of transparent sample.

The critical indices β have been calculated on the basis of spontaneous increases of the values $\Delta Y_s(T)/\Delta Y_s(T_{min})$ experimentally measured. Here $T < T_c$=49°C and T_{min}=39°C. The values of Y are optical retardation ($Y = \Delta$), geometric thickness ($Y = l$), and susceptibility ($Y = \eta$).

Deviation of the critical indices β of TGS from the unity ($\beta = 0.87\ldots0.95$) has been explained by significant temperature dependence of coefficients of the electrostriction and the inverse piezooptic effects of maximum-like character in the temperature range around T_c of the crystal.

Various relations between the critical indices on linear deformations $\beta^{(l)}$ and on susceptibility $\beta^{(\eta)}$ for the direction of spontaneous polarization [010], $\beta_2^{(l)}(\eta)$, and for two other less symmetric directions [100] and [001], $\beta_{1,3}^{(l)}$(l)> $\beta_{1,3}^{(n)}$, testify for various rates of temperature changes of different subsystems, taking place in ferroelectric ordering of the crystal in the temperature range (ΔT ˜ 10°C) below the PT point. Different β-values lead to the temperature dependences of the relative changes of $\Delta Y_s(T)/\Delta Y_s(T_{min})$, which can be characterized by different derivatives at different temperatures.

Relaxation dynamics of disordered Ising-like models

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Two-site cluster approximation to Glauber's master equation is developed for lattice spin systems with substitutional chaos. Quenched and annealed types of disorder are considered. The order parameters and the dynamic pair correlation functions of disordered Ising and Mitsui models are calculated. The agreement between the theory and results of the dielectric measurements in the ferroelectric crystals $Cs(H_{1-x}D_x)_2PO_4$, $Rs_{1-x}dRs_x$ (Rochelle salt) is remarkably good. The theory suggests the strong tendency to alternation of protons and deuterons to exist in the H-bond chains of $Cs(H_{1-x}D_x)_2PO_4$ crystals. Since the isotope effects in the Rochelle salt are much less pronounced and few measurements in the partially deuterated crystals have been performed, we can not currently detect the type of disorder in $Rs_{1-x}dRs_x$.

Doped molecular crystals as erasable optical information storage

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Possibility of the hydrogen bonding between impurity and host molecules promotes variety of the different positions and orientations of the impurity molecule. This effect is especially pronounced for aromatic host molecules which act as planar and extended proton acceptor. Light irradiation causes reorientation of the impurity molecule and breakdown of the hydrogen bonds [1]. It leads to the complete and long-lived changes of the impurity absorption spectrum. In order to restore initial impurity spectrum the long-term annealing is necessary. The parameters of the observed phototransformations (temperature and exposure, which are necessary for the complete changes) depend on the molecular structure of the impurity and host molecules [2].

In order to find mechanism of these phototransformations the possible structures of the impurity centers in the ground and excited states were calculated using method of the atom-atom potentials. In the ground state the set of the possible impurity sites, with and without hydrogen bonds, was found. If the impurity contains aminogroup, the sites with one or two hydrogen bonds are possible. Usually the sites with hydrogen bonds are energetically preferable. It was found that optical excitation of the states with charge transfer between impurity and host molecules causes breakdown of the hydrogen bonds [3]. This effect takes place if the ionization potential of the impurity is lower in comparison with host molecule. The efficiency of the phototransformations increases with the decrease of the impurity size.

The obtained results allow to propose the doped molecular crystals with hydrogen bonds as promising media for the erasable optical information storage. From a knowledge of the mechanism of the observed phototransformations their parameters can be varied purposefully by the change of the molecular structure of the components.

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Hall effect in disordered transition metals

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How does one extract many-body interatomic potentials from ab-initio band structure calculations?

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An original method to treat the kinetic and exchange-correlation energy functionals in terms of many-particle interactions has been developed. It is based on utilizing of the local density approximation. The total electron density, extracted from the ab initio band structure calculations, is expressed as a linear superposition of contributions from the individual pseudoions embedded in the uniform background. The general form for the part of effective interatomic interactions caused by the kinetic and exchange-correlation effects is obtained. Relationship between the developing approach and the perturbation theory in pseudopotential is analysed. Unlike the perturbation theory, the presenting method allows one to work out in a general form a procedure for renormalization of the n-particle irreducible interactions by the $(n+1)$-, $(n+2)$- etc. reducible ones. Such a renormalization of the pair interatomic potential is given.

Contribution of the electron-nonlocal pseudopotential interactions to the pair interatomic potential is considered within the concept of the full separable pseudopotentials. The explicit expression for the three-particle interatomic interactions is also presented.

Influence of ions on the critical behaviour in liquid mixtures near critical solution point

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Recent investigations of the critical behaviour in ionic mixtures rose a problem of the connection of the critical parameters (critical temperature, concentration) and the critical properties (their critical exponents and amplitudes) with the solution structure and intermolecular interaction in the solution. The ionic impurities strongly influence on the molecular structure of aqueous solutions of organic molecules and shift the upper and lower critical solution temperatures. The sensitivity of the critical temperatures to ions depends on the anions and cations as well as on the organic solute. The recent experimental results on the influence of ions on the critical properties, i.e. on critical exponents, nonuniversal critical amplitudes, asymptotic and crossover ranges are analysed. The interpretation of experimental results based on the clustering in solution is proposed.

Posters

BBGKY–hierarchies for equilibrium state of the weakly relativistic systems of the charged particles

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The charges system with Coulomb and electromagnetic interactions, described by Darwin's Lagrangian is considered. On the basis of Lagrange's and Hamilton's approaches the equilibrium Gibbs distribution, BBGKY–hierarchies as well as one–body and two–body distributions are obtained. The influence of external stationary electromagnetic field and many-particle character of electromagnetic interaction are taken into account. This allowed to regularize atoms of relativistic long–range divergencies in natural way. The existence of collective self–action effects of charges provides the obtaining of correct quantitative results and is connected with peculiarities of regularization procedure in relativistic statistical theory of charged particles systems. It is shown that these effects lead to the renormalization of many particle distribution functions, that can be considered in weakly uniform case as the result of the appearance of the effective mass of particles. In this case the essentially manyparticles character of the electromagnetic interaction displayed itself in the form of relativistic screening effects too.

Multipole expansions and relativistic long–range effects in statistical theory of many atom systems

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The system of atoms with taking into account the retardation interaction effects is considered. On the basis of generalization of Breit Hamiltonian in the case of dynamical polarization of medium, the Hamilton's operator, describing multipole interactions of atoms with taking into account the relativistic long–range corrections is constructed. Because of this generalization it turns out to describe correctly the interaction of atoms as well as large and not very small distances.

The influence of relativistic corrections on dipole and van der Waals interactions of atoms is considered in details. It is shown that in some cases these corrections can be commensurable or even more essential then the main nonrelativistic contributions.

Tensor of dielectric permittivity of weakly relativistic plasma

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The weakly relativistic system of charged particles with spins in the external electromagnetic field is considered. Besides Coulomb and magnetic interactions, the spin–spin, spin–orbital and contact interactions are also taken into account. "Mixed" representation of statistical operator in the form of regularized path integral for coordinate degrees of freedom and simple exponent operator for spin degrees of freedom is proposed. The weakly relativistic Hamilton function is obtained in random phase approximation. The screening of the interaction of charges with magnetic field is proved. The thermodynamical potential of the system and temperature Green functions for correlations "density–density" and "current–current" are calculated. Obtained results are used for finding of dielectric permittivity tensor of relativistic electron gas. Numerical calculations of static dielectric and magnetic permittivities of completely degenerated and high–temperature electron gas are carried out. The contributions of certain relativistic effects like kinematic corrections, corrections to Coulomb and spin interactions are analysed. Separately, for dielectric permittivity it is shown that for big values of wave vector the contributions of relativistic kinematic and spin effects mutually reduce. For long range the intensity of spin interactions decreases and kinematic effects predominate. In general, the accounting of spin interactions drives to decreasing of total relativistic correction for thermodynamical functions, as well.

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The dielectric permittivity of non-polar system in the Random Phase Approximation

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The dielectric properties of non-polar condensed matter are investigated. To find a polarization of the system, the dipole moments of particles, induced by non-uniform electrostatics field are obtained. The effects caused by the long-range dipole interaction are taken into account in the Random Phase Approximation (RPA). It is shown that the effects of the long-range interaction can be taken into account by renormalizing the polarization of separated particles (α). The vector of the polarization is defined by functional differentiation of grand partition function (Q_N) of dielectrics. To calculate Q_N the expansion

$$Q_N = 3DQ_1^N(1 + Nb_2 + N^2b_3 + \ldots)^N$$

is used, where N is number of particles and $b_2, b_3, \ldots$ are defined via virial coefficients. For dielectric permittivity we have obtained the analogue of Clausius-Mossotti's formula with renormalized polarization (α^*), which is defined by relationship

$$\alpha^* = 3D\alpha\left\{1 + 2\rho^*\frac{\alpha^2}{(1-\eta)(1+2\eta)}\int\frac{d^3x}{x^6}e^{-\Phi(x)/\Theta},\right\}$$

$$\rho^* = 3D\rho\left[1 + 2\pi\frac{N}{V}\int_0^\infty dxx^2(e^{-\beta=20\Phi(\mathbf{x})}-1)\right]^{-1}, \quad \eta = 3D\frac{4\pi}{3}\rho\alpha$$

where ρ is the density, $\Phi(x)$ is the energy of interaction in absence of external field and Θ is statistical temperature.

The effectiveness of the results obtained is illustrated on the example of the system of particles with Lennard-Jones interaction and different values of density, polarization and temperature. A comparison with the Molecular Dynamic (MD) results and other works is carried out.

The generalization of reference system approach to the case of relativistic Fermi-systems

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The extended before statistical reference system approach for the non-relativistic quantum systems [1, 2] is generalized to the case of relativistic Fermi-systems. The peculiarities of n-particle dynamical corrrelation functions of the reference system (ideal degenerated Fermi-system) are studied. It was done for the case of low temperatures and arbitrary value of relativistic parameter $\gamma_F = v_F/c$ (v_F is the velocity of the particle on the Fermi surface, c is the light velocity)

$$\begin{aligned} &\mu_n^0(x_1, ..., x_n|\gamma_F, \beta) = \beta^{-1}\langle T\{\hat\rho_{x_1}\hat\rho_{x_2}...\hat\rho_{x_n}\}\rangle_0, \\ &\hat\rho_x = \sum_{\mathbf{k},s,\nu^*} a^+_{\mathbf{k}+\mathbf{q}}(\nu^*+\nu)a_{\mathbf{k},s}(\nu^*), \\ &a_{\mathbf{k},s}(\nu^*) = \beta^{-1/2}\int_0^\beta d\beta^{'}\exp(i\nu^*\beta^{'})a_{\mathbf{k},s}(\beta^{'}). \end{aligned} \tag{1}$$

Here $x \equiv (\mathbf{q}, \nu)$, $\mathbf{q}$ and $\mathbf{k}$ are the wave-vectors, s is the spin variable, ν and ν^* are Bose-Matsubara and Fermi-Matsubara frequencies, respectively, T is the symbol of chronological ordering, β is the reciprocal temperature, symbol $\langle...\rangle_0$ means the statistical averaging over the reference system states, $a_{\mathbf{k},s}(\beta^{'})$ is the secondary quantization operator in the plane waves basis in the interaction representation.

The pattern of integral equations of the second order Fredgolm-like type for the local field correction function of relativistic Fermi-system was obtained. The solutions for the electron system at the weak nonideality over the parameter γ_F were investigated. On this basis thermodynamical and structural functions for the relativistic electron system with Coulomb interaction at the small values of Vigner-Brueckner parameter r_s and arbitrary values of γ_F were calculated.

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The modificated displacements method in the Fermi-liquid and metals theories

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For the investigation of strong coupled Fermi-systems a new version of displacements representation for statistical operator

$$\hat{R} = \exp\ [-\beta(\hat{H}_0 + \hat{V} - \mu\hat{N})] = \{\exp\ \hat{U}\}\ \hat{\sigma}, \tag{1}$$

is proposed. Here $\hat{H}_0$ is the kinetic energy operator, V is the interaction operator, $\hat{N}$ is the number of particles operator, μ is the chemical potential variable. It was proved that for the low temperatures the displacements representation is equivalent to cyclic transformation of partition function:

$$Z = \mathrm{Sp}\ \{\hat{R}\} = \mathrm{Sp}\ \{\exp\ [-\beta e^{-\hat{U}}(\hat{H}_0 + \hat{V} - \mu\hat{N})e^{\hat{U}}]\}. \tag{2}$$

Different choice variants of displacements operator $\hat{U}$ correspond to different renormalized perturbation theories, in which a weak effective interaction potentials is present. It makes possible the natural way accountment of screening and local field effects. For the calculated ground state energy of electron liquid model in the wide region of coupling parameter ($10^{-2} \le r_s \le 10$) a good agreement with the results of Monte-Carlo method are obtained. For this model the pair distribution function and the local field correction were calculated too.

The displacements representation was generalized on the case of electron-ionic metal model as with local as with unlocal electron-ionic interaction potentials. Two different variants of theory are proposed. In the first one the displacements representation was adopted for the reference system description (electron liquid model). In the second variant the displacements representation is used for the description of collectivized electron subsystem in the ionic field. The calculated potentials of effective ion-ion interaction are in good agreement with the results obtained in the local field approximation and the bonding energy of metal – with the experimental data.

Investigation of the electron liquid model at nonzero temperatures

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Calculation of the thermodynamical characteristics for the systems of interacted fermions at nonzero temperatures is vital problem of the statistical physics.

In this paper we investigate characteristics for the electron liquid model at nonzero temperatures. All calculations were carried out in the frame of a reference system approach - the renormalized perturbation theory, which is formulated in terms of n-particle correlation functions $\mu_n^0(x_1,\ldots,\ x_n|\mu)$ ($x_i \equiv (\bar{q}_i, \nu_i)$) of some simpler model system, called the reference system. Model of the free electron gas was chosen as a reference system.

For the first time, the n-particle dynamic correlation functions $\mu_n^0(x_1,\ldots,x_n|\mu)$ at $T^* \equiv T\,(k_B\epsilon_F)^{-1} = 0$ were investigated in [1].

We propose the method for calculation of the temperature correction $\delta\mu_n^0(x_1,\ldots,x_n|\beta,\mu)$ to n-particle dynamic correlation functions $\mu_n^0(x_1,\ldots,x_n|\mu)$, and study features of $\delta\mu_n^0(x_1,\ldots,x_n|\beta,\mu)$ for the case $n = 2, 3$.

On this basis thermodynamical characteristics of the electron liquid model at nonzero temperatures have been calculated in the weak and medium nonideality region. Results for free energy, chemical potential, heat capacity were compared in the different approximations.

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Fluctuational dynamics and structure factor of nonlinear reactive systems on a 1D lattice

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Within the investigated model of one-dimensional bi- and tri-molecular chemically reacted crystal the asymptotic behaviour of amplitude of two-particle static structure factor (as a function of crystal length) has been discovered. The nonlinear fluctuational scenario which is mentioned gives rise to conclusion of the principle possibility of existence of the asymptotic metastable cluster fragmentation within the initially homogeneous 1D systems. There was obtained an experimental indications of the existence of the metastable states in form of clusterisation in rare gas cluster ions initiated by eximer decay [1,2]. Because of the important role of size and dimensionality in the development of nonlinear chemical dynamic scenario within the chemically reacting systems and due to intensive experimental investigation of the clusters from the small number of particles new specific effects in scattering are also reported [1-3]. The connection between some possible effects and the properties of the fluctuations in the above reacting systems and reactive dynamics in a partially filled lattice is also performed.

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Tamm's resonances and minibands within the model one-dimensional potential

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The modelling of low-dimensional atom-molecular complexes, adatomic clusters, chains, lattices and superlattices belong to a number of traditionally and actively considered problems of the solid state theory [1,2]. The urgency of that exploring is limited by the essentiality and the difficulties of direct microscopic description of the synthesized in the recent time low-dimensional atom-molecular complexes and other physical objects with the symmetry. On this way, in particular, in [3] one-dimensional Kronig-Penny superlattice with the regular intrinsic structure determined by the combination of zero-radius potentials [4] was studied. Then the simple analytical model permitting to explore some general properties of superlattices and separate contacts (interfaces) being the model elements for the description of semiconductor and metallic films, quasicrystalls and other same objects is suggested [2,5]. Such a model can be used in the construction of more common theories. In this paper with the help of transfer-matrix formalism the problem about regular superlattice's spectrum is considered and a simple method of description of the contact in the superlattice's structure is suggested. It is shown the existence of the single contact induce of the separate pair resonances in the chain's spectrum (which are distributed in the permitted and the forbidden zones, respectively). Also it is demonstrated the eroding of noted minizones after making connection between the separate regular segments in the superlattice. The similar resonances and minizones can be called the Tamm's ones being useful elements for the description of the surface states and zone-band structure of real low-dimensional systems.

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Screening potentials and cluster expansions of ionic-molecular systems adsorbed in dielectric disordered matrices. Application of replica Ornstein-Zernike equations

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A. Given and G.R. Stell [1] have proposed the replica Ornstein-Zernike equations for fluids in porous medium. In [2] this techniques was used for description of screening of ion-ion correlations in electrolyte solutions adsorbed in electroneutral disordered matrices of charged particles. Recently, we applied it to calculation of screening potentials of ion-molecular systems adsorbed in dielectric disordered matrices. We show that screening by the dielectric disordered matrix introduces a dielectric constant ε_0 to screening potentials interactions between particles of fluid and particles of matrix. Connected part of ion-ion of screening potential is independent from matrix, whereas blocking part of ion-ion screening potential includes the parameter $(1-\varepsilon_0)/\varepsilon_0$. We have analysed in details screening potentials for three type of fluids adsorbed in dielectric disordered matrix (1. ionic fluid, 2. dipole fluid, 3. ion-dipole fluid) [3]. The obtained screening potentials are used for the construction of the cluster expansions of the correlation functions.

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Some aspects of applying the associative theory to the self-ensemble system

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The system which consists of water and amphiphiles (surfase–active particles) is considered. The aggregates of different size and form (called as micelles), which are the simplest example of the self–ensemble system, can start to create at the certain concentration of amphiphiles. This concentration is called as the certain (or critical) micell concentration (CMC). Usually the CMC can be found from the mass action law by thermodynamical methods (in assumption of ideal gas mixture of micelles created).

In contrast to the above approach we propose the model of the system with associative interaction between the amphiphiles. We use this model to describe the system in which only one–dimensional (e.g. spherocylindrical) micelles appear. The grand partition function can be written as

$$ln\mathcal{Z} = ln\mathcal{Z}_1 + \sum_G \mathcal{F}_G,$$

where G is the geometrical factor of micelles created. Taking into account only the chain form of micelles $G = C$ and using

$$\rho = \frac{z}{V}\frac{\partial ln\mathcal{Z}}{\partial z},$$

the expression for amphiphile concentration ($X = N_a/N_{tot}$) can be expressed as

$$X = X_1 + \frac{2JX_1 - (JX_1)^2}{\rho_{tot}(1-JX_1)^2},$$

where J depends on ρ_{tot}, size, interaction and correlation functions. The concentration $X_1 = 1/J$ is treated as the CMC.

The structural properties of the system studied can be found by using Ornstein–Zernike equation. The attempt to generalize our method to many–componet systems has been done.

On the effects of association in the statistical theory of ion-dipole systems

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We discuss our recent results [1] in the statistical theory of association effects in ion-dipole systems. We believe that associations can occur due to strong electrostatic interactions and by the chemical association mechanism is which the a true chemical bond is formed. The associative mean spherical approximation (AMSA) for a mixture of polar hard spheres and charged hard spheres is solved in the multidensity formalism. Analytical results for thermodynamic quantities (the Helmholz free energy, chemical potential and pressure) and dielectric constant are expressed in terms of the excess internal energies, which follow from the solution of a set of algebraic equations. The method of derivation is based on the extension of Hoye-Stell scheme [2] in the frames of the multidensity formalism and exponential approximation proposed by Bernard and Blum [3]. This technique was recently suggested by Kalyuzhnyi and Holovko [4]. We investigate the influence of ion-ion, ion-dipole and dipole-dipole associative interactions upon the thermodynamic and dielectric properties. It is shown that the dielectric constant increases with the increase of the ion-ion association strength parameter. The ion-ion, ion-dipole and dipole-dipole pair correlation functions are obtained by the iteration scheme of Perram [5].

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Critical phenomena in ionic ferrocolloidal model

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Ionic ferrocolloids are aqueous dispersions of the magnetic particles with surface charge which ensure their stability. We consider the model in which the particles are represented by the polyions with the additional magnetic dipole moment. In order to satisfy the electroneutrality conditions the ions of the opposite sign (counterious) are also taken into account. Both kind of the ions are chosen to be the hard spheres with strong asymmetry in sizes and charges. In addition it is assumed that pair potential acting between ions includes also van der Waals type of interaction. Free energy is presented as a sum of four terms: hard spheres contribution, which is described using Carnahan-Starling approach; contribution of the van der Waals attractive interaction, which is described in the frames of the molecular field approach; ionic contribution which is calculated by means of random phase approximations. Description of bonding effects between counterious and polyions is carried out in the multidensity associative formalism. Dipole-dipole interaction is divided into long- and short-range parts. The long-range part of the dipole-dipole interaction is calculated using Pade approximation method. For calculation of the short-range part of dipole-dipole interaction all chain diagrams are summed and treated in the two-density associative formalism. The influence of different interactions on the critical behaviour of the gas-liquid like phase transition is discussed.

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Dipolar hard spheres with orientationally-dependent association interaction

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The multicomponent dipole model with arbitrary sizes and dipole moments of particles is considered. All the species present in the mixture may have associative interactions with dipolar symmetry. For the description of this model we (together with Prof. M.Holovko) have studied the associative mean spherical approximation. For the solution of the problem a Baxter factorized version of the Wertheim-Ornstein-Zernike equations and the technique of Blum and co-workers were used. The description of the orientational dependence in the interparticle potential was carried out using expansions in terms of generalized spherical functions. The expressions for the factor correlation functions are presented.

Investigation of triple $K + K^{+0.5} + O^{-1}$ system by MD method and statistical geometry

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The molecular-dynamic simulation of potassium/oxygen system evolution was made for investigation the impurity influence. The liquid potassium/oxygen system was considered as model of triple system $K + K^{+0.5} + O^{-1}$ in condition of total neutral of system. Potassium particles ionized as the twofold concentration of oxygen in mixture. Oxygen was as oxide microinclusions with mass density $\rho_{K_2O} = 2320\ kg/m^3$ at a given oxygen atomic concentration of 8.5%. The mass density of liquid potassium is $\rho_K = 777\ kg/m^3$. The simulation has been fulfilled at temperature 550K in the frame of NVT ensemble for the model of N=3456 particles including 294 oxygen ions O^{-1}, 588 potassium ions $K^{+0.5}$ and the rest of neutral potassium atoms. The generalised form of interatomic pair potential (Lennard-Jones n-m potential) is used for (K,K) and (K,K^+) interaction and Born-Mayer potential without dispersion terms is used for (K^+, O^-), (O^-, O^-) and (K,O^-) interactions.

The evolution of characteristics of potassium/oxygen system such as the partial radial distribution functions, $g_{\alpha\beta}(r)$, structure factors, $S_{\alpha\beta}(k)$, velocity autocorrelation functions, $\Psi_{\alpha\beta}(t)$, frequency spectra, $f^n_{\alpha\beta}(w)$, and self-diffusion coefficients, $D_{\alpha\beta}$, has been examined up to $5.7 \cdot 10^{-11}$s. The addition analysis of atomic configuration in time t_i has been performed upon the basic of Voronoi-Delaunay division of space into polyhedra. The observed structural and dynamic changes of potassium/oxygen unordered system reflect the process of admixture behaviour and in particular the process of atomic clusterization in liquid alkaline metals.

Exactly solvable models of anisotropic fluids with long-range pair potentials

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It is generally accepted that the Onsager system of long hard spherocylinders is the only exactly solvable model of anisotropic fluids. But the excluded volume models (including the Onsager model) is of little value for thermotropic liquid crystals. Therefore, the search of exactly solvable models with long-range pair potentials is of great importance. We consider models of anisotropic fluids with the pair potential containing contributions from a hard core and a long-range interaction of type $\gamma^3 f(\gamma R_{12}) P_l(\cos\omega_{12})$, $P_l(\cos\omega_{12})$ is the lth order Legendre polynomial of the relative molecule orientation, $\gamma^3 f(\gamma R_{12})$ is a Kac potential. On the basis of the collective variables and the integral equation methods the existence of thermodynamic limit for the model free energy in the anisotropic phase is proven. The exact and finite series are written for the free energies of such models with hard core interactions in the form of the Onsager spherocylinders or the hard spheres. In contrast to the well-known Onsager model these exactly solvable models describe the orientational phase transitions that are dependent on temperature. The phase diagrams of such models are shown.

Model description of the H–bonded transuranium complexes

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Presented report includes the part of results obtained in the framework of INTAS–Ukraine–95–0133 project “Investigation of the complex formation and ionic transport processes in water, aqueous solutions and H–bonded systems for the development of environmental protection solutions connected with water pollution”.

The approach based on the pseudospin formalism for the description of the molecular and ionic complexes as well as chain–like H–bonded structures with highly valent transuranium elements is presented.

Model of the polymerization of ionic groups UO_4 into chain structure via hydrogen bonds is proposed. The conditions of the thermodynamic stability of such formation are investigated in dependence on number of links at different temperatures and pH values of solution.

The process of formation of hydroxocomplexes in such systems is considered. For the investigation of equilibrium between H–bonded transuranium oxide complexes and hydroxocomplexes the thermodynamics of repolarization due to the proton transfer in the hydrogen bonds is described. The expression for equilibrium constant is obtained.

Microscopic consideration of the complex formation of actinide group ions in the aqueous solution is carried out on the base of configurational description. The calculation of the creation probability of complexes $[\mathrm{M(OH)}_n\mathrm{H}_m]^{(Z-n+m)}$ is performed in dependence on the configuration energy, temperature and chemical potential of groups $(\mathrm{OH})^-$ and ions H^+ in solution with small values of pH. The attention is paid on the saturation effects at increasing of concentration as well as on the transformation processes between equilibrium configurations of complexes.

The reduced basis model for H–bonded one–dimensional molecular systems [1] is generalized for the charged systems.

The possibility of application of the orientational–tunnelling model [2] for the description of the tritium migration mechanism is discussed.

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Investigation of the electronic properties of the hydrogen bond

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The properties of the hydrogen bond are investigated on the basis of the simplest object with hydrogen bond, the ionic complex O-H-O. The electron energy spectrum of the O-H-O complex with account of Coulomb and exchange interactions as well as an electron transfer is obtained. The formation of the two-minima adiabatic proton potential as a function of the hydrogen bond length R_{OO}, R_{OH} distance, electron number N on complex is investigated. It is shown that the decrease of the number of electrons on the cluster leads to the increase of the critical value R_{OO}^{cr}, at which the double minima potential well transforms into single minimum one. The electron density maps and the distribution of the electron charge along the complex axis are obtained. We investigate also the change of the electron charge density and the occupancy of the atomic orbitals of the initial basis connected with proton shift along hydrogen bond. Proton shift on a bond is accompanied by the increase of the total electron density in the region where the proton is moved to; however, the occupancy of the 2p-orbitals of the corresponding oxygen ion is decreased. Occupancy of 1s-orbital of hydrogen ion changes weakly and possesses maximum at the location of proton in the middle of the bond. That is in agreement with the experimentally obtained results.

Such calculations for the cluster with few hydrogen bonds allow to investigate the connection between electron density changes and proton-proton short range interaction. Describing systems with hydrogen bonds using different models one should take into account these interactions. More detailed study of this problem will give an opportunity to formulate more realistic models for description of such objects.

Correction of finite-size effects in molecular-dynamics simulation of liquid alloys

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The fixed number of particles in computer simulations produces systematic and random statistical errors in the long-range region of the pair distribution functions. These in turn lead to significant uncertainties in the static structure factor in low-Q region.

We present a method for a finite-size correction in the calculation of the partial pair distribution functions and static structure factor of binary liquids from MD simulation data. The method is based on the combined using of a theoretical O(1/N) correction of $\mathrm{g}_{ij}^{N}(\mathrm{r})$ for a N-particle system and MHNC integral theory. The proposed method is used for the analysis of MD simulation data for a liquid $\mathrm{Na}_{0.7}\mathrm{K}_{0.3}$ alloy. The simulations were performed for two system sizes N=500 and N=2048 particles. It is found a good agreement between the $\mathrm{g}_{ij}^{N}(\mathrm{r})$ and S(Q) obtained from MD simulations with the predictions of MHNC theory. In addition we have calculated the bridge functions $\mathrm{B}_{ij}(\mathrm{r})$ from $\mathrm{g}_{ij}^{N}(\mathrm{r})$.

Single-particle motion in liquid and supercooled $Mg_{70}Zn_{30}$ alloy

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We report the results of a self-consistent mode-coupling (MC) calculations of the velocity autocorrelation functions (VAF) of both species and the corresponding memory functions for liquid and supercooled $Mg_{70}Zn_{30}$ alloy. The static structure required for the theoretical study have been obtained by combined using of molecular-dynamic simulation and integral-equation technique.

In the framework of MC theory the memory function for the VAF is split into two contributions: a short-time part is described as the effect of single uncorrelated binary collisions and a long-time 'mode-coupling' contribution is represented in terms of non-linear couplings of slowly varying collective variables. In present calculations we used a simple Gaussian *ansatz* for the 'binary' part of the memory function and coupling with density fluctuations for the mode-coupling component. The intermediate scattering functions, involved into the mode-coupling integral, are calculated in the viscoelastic approximation whereas the incoherent scattering functions are calculated self-consistently, from the obtained VAF.

We compare the results of MC calculations with those directly obtained from MD-simulation.

Spectra of transverse excitations and reduction of hydrodynamic region in glassforming metallic liquid alloy $Mg_{70} - Zn_{30}$ by approaching the transition temperature

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The method of generalized collective modes (GCM) has been applied for the investigation of dynamical properties of glassforming metallic system $Mg_{70} - Zn_{30}$ in three different liquid states. This approach allows to solve the generalized Langevin equation in Markovian approximation and to decompose time correlation functions derived in molecular dynamics into partial contributions associated with eigenmodes of system investigated. In our calculations the Markovian transverse 'current-current' time correlation functions have been obtained within the four-variables approximation and satisfied the sum rules up to the frequency moment of sixth order.

Applying the approach of GCM to dense metallic binary system $Mg_{70} - Zn_{30}$ we were able to obtain without any fitting parameters the spectra of transverse collective excitations and to estimate the boundary of hydrodynamic region $k_H(T)$, in which the lowest-lying pair of propagating modes disappeared transforming into two relaxing modes. For $k > k_H$ those propagating modes described transverse shear waves observable in the behaviour of 'current-current' time correlation function. When $k < k_H$ one of the relaxing modes in the hydrodynamic limit had the eigenvalue proportional to k^2 with the coefficient $\eta(T)/\rho$ (η and ρ were shear viscosity and mass-density, respectively), while the second one was the relaxing kinetic mode. The width of hydrodynamic region became narrower by decreasing the temperature and at approximately 80K above the experimental eutectic temperature we found it to be extremely small.

The generalized shear viscosity as a function of wave-vector for a liquid metallic binary system has been calculated for three temperatures: from a 'good' liquid system to a system close to the glass transition. Obtained values of shear viscosity at those temperatures could be compared with experimental data.

A new approximate procedure for memory function calculations: generalized shear viscosity and the "shoulder" problem for a simple fluid

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For approximate calculations of memory functions in a wide range of wavenumbers k and frequencies ω a new iteration scheme based on recurrent relations for higher order memory functions is developed. Within this scheme memory functions can be presented in an analytical form and their k-dependence is formed only by higher order static correlation functions which are the main input of the theory. As an illustration we consider the application of the scheme for the study of generalized shear viscosity $\eta(k, \omega)$ of a Lennard-Jones fluid where traditional approaches have shown a systematic deviation from molecular dynamics (MD) data, in particular, in the range of intermediate values of k, where some peculiarities in k-behaviour of $\eta(k)$, known in the literature as "shoulder" problem, were found.

By the numerical calculations it is shown that the iteration scheme has a tendency for the convergence of the results when the order of approximations increases, but even the first approximations describe well the generalized shear viscosity for all the wavenumbers considered herein, starting from the hydrodynamic values and up to so-called Gaussian limit. The obtained results are in a good agreement with MD data. The proposed approach can be also used for the study of other physical systems.

Statistical hydrodynamics of a multi-component mixture: Generalized mode approach

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Using Zubarev's non-equilibrium statistical operator the statistical theory of a weakly non-equilibrium multi-component, chemically nonreactive mixture of simple liquids is developed in the most general form. The basic equations of generalized hydrodynamics are derived. We find the explicit expressions for the generalized thermodynamic quantities and the generalized transport coefficients and show that in the hydrodynamic limit the results known previously in the literature are reproduced. For an extended set of dynamic variables, including in addition to the operators of conserved quantities their higher order time derivatives, the recurrent relations for the memory functions are derived. All the results are presented in the form allowed directly to apply the generalized mode approach for the subsequent calculations of generalized collective modes spectrum, time correlation functions and generalized transport coefficients as well. We illustrate our theoretical study by the numerical results obtained for binary mixtures of He-Ne and He-Ar. Particular emphasis will be placed on a discussion of generalized propagating kinetic modes to be observed experimentally.

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A new approach to the numerical integration of the rigid-body equations of motion

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The method of molecular dynamics plays a prominent role in study of molecular liquids. Existing techniques appropriate to simulate such systems can be categorized in dependence on what type of parameters are chosen to represent the rotational degrees of freedom and what kind of numerical algorithm is applied to integrate the corresponding equations of motion. There is a group of stable algorithms to integrate numerically the equations of motion on rigid polyatomics. However, in these approaches to reproduce the rigid molecular structure it is necessary to solve by iteration complicated systems of nonlinear equations at each time step of the integration.

In the present investigation we propose a new algorithm for numerical integration of the rigid-body equations of motion. The main idea consists in involving angular velocities, instead of angular momenta, into the integration. The orientational variables are expressed in terms of either principal axes or quaternions. This leads to a very powerful technique, because the orthonormality and unit norms of orientational variables appear to be integrals of motion, despite an approximate character of the produced trajectories. Therefore, no additional efforts are needed to preserve the rigidity of molecules. Moreover, no iterative solutions are necessary in our scheme at all.

The algorithm introduced might become popular because of its excellent stability, simplicity to implement for arbitrary rigid bodies and its intrinsic conservation of rigid structures.

Statistical hydrodynamics of a binary ferromagnetic mixture

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In this report the generalized hydrodynamics of mixture of magnetic and nonmagnetic liquids is studied. Using the nonequilibrium statistical operator method, the equations of generalized hydrodynamics for conserved quantities, namely, for the densities of energy, total momentum, particles' numbers for magnetic and nonmagnetic subsystems, and magnetization, are derived. The magnetic subsystem is described by a Heisenberg-like model. The microscopic expressions for the generalized k-dependent thermodynamic quantities and the generalized (k, ω)-dependent transport coefficients are found.

In the hydrodynamic limit the collective mode spectrum is obtained. We find two complex-cojugated sound modes and three (heat, diffusion and spin diffusion) relaxing hydrodynamic modes. The hydrodynamic time correlation functions, constructed on conserved variables, as well as the weight coefficients describing a partial contribution of each from the modes to all the hydrodynamic time correlation functions, are calculated by the means of matrix perturbation theory for the hydrodynamic operator.

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Study of nonlinear hydrodynamic fluctuations of super dense plasma

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We investigate nonlinear hydrodynamic fluctuations of super dense electron plasma ($n_e \sim 10^{21} \div 10^{22}$ cm^{-3}, $n \sim 10^{25} \div 10^{26}$ cm^{-3}), which is created at laser nuclear fusion of D-D, D-T, D-^{3}He mixtures [1,2]. Electron and ion densities in processes of action of powerful spherical short-wave laser irradiation as well as target ablation and implosion enlarge ten up to thousand times. Such densities correspond to liquid and super hard core ones. It is obvious, that gas dynamics methods of description of transport processes, where the one-particle nonequilibrium distribution function is a basic parameter of enshortened description, is rough and very approximate and can not be applied in principle. Moreover, in super dense plasma the influence of a potential interaction energy is considerably larger than the kinetic one. It reflects essentially on thermal conductivity processes of both electron (corona) and ion (core) subsystems. Considering these facts, generalized equations of nonlinear hydrodynamics for super dense electron-ion plasma have been obtained using the nonequilibrium statistical operator method [3,4] with taking into account a self electromagnetic field generation. During the synthesis in the centre of nuclear fuel to be compressed up to ignition temperature interaction potentials of ions D, T, ^{3}He have a nuclear quark-gluon nature of proton and neutron interactions.

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A model for radionuclide migration with ground water

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The object “Shelter” at Chernobyl nuclear power plant contains a lot of radioactive materials. Aqueous medium increases their mobility so dangerous elements are persistently penetrating into environment with ground water. Recent measurements show there are above 3000 m^3 of water at the object, only 1000 m^3 being under control. The egress is supposed to have a diffusion nature.

The model for diffusion treatment of active elements migration with ground water is proposed on the basis of two phase system “aqueous radioactive solution-clayey ground”. Within this model active elements particles (UO_2^{2+}, Cs^+, Sr^{2+}) are considered as charged hard spheres having the overall charge to be compensated according to the electroneutrality condition by negative OH^--groups in a continuous medium with the dielectric constant $\varepsilon_p = 81$ (water). The second phase is a continuous medium with the dielectric constant $\varepsilon_c = 1 \div 15$ (clay). Effects of electrostatic images are taken into account.

Diffusion coefficients are derived from the nonequilibrium statistical mechanics. They are expressed through singlet and pair equilibrium distribution functions to be evaluated for radioactive particles in the above mentioned model at various concentrations. Expressions for diffusion coefficients reduce to those obtained by other authors earlier for the homogeneous case.

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Transverse dynamics of spin-$\frac{1}{2}$ XX chain in transverse field with correlated Lorentzian disorder

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We consider spin-$\frac{1}{2}$ XX chain in transverse field governed by the Hamiltonian

$$H = \sum_{n=1}^{N} \Omega_n s_n^z + \sum_{n=1}^{N-1} J_n (s_n^x s_{n+1}^x + s_n^y s_{n+1}^y)$$

with random independent Lorentzian exchange couplings centered at J_0 with the strength of disorder Γ and transverse fields that depend linearly on the neighbouring couplings

$$\Omega_n - \Omega_0 = a \left(\frac{J_{n-1} - J_0}{2} + \frac{J_n - J_0}{2} \right).$$

Thermodynamic properties of the model can be obtained analytically for $\mid a \mid \geq 1$ [1]. We studied transverse dynamics of the model computing numerically [2] the correlation functions $\langle s_j^z(t) s_{j+n}^z(0) \rangle$ and therefore the dynamic structure factor $\overline{S_{zz}(\kappa, \omega)}$ and susceptibility $\overline{\chi_{zz}(\kappa, \omega)}$. We discussed in detail the effects of correlated disorder comparing the results with the corresponding ones for the model with independent Lorentzian exchange couplings and transverse fields.

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Thermodynamic properties of nonuniform spin-$\frac{1}{2}$ XX chain in transverse field

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We consider a nonuniform spin-$\frac{1}{2}$ XX chain in transverse field that due to the Jordan-Wigner transformation can be viewed as one-dimensional nonuniform system of noninteracting fermions. For any periodic configuration of exchange couplings J_n and transverse fields Ω_n the temperature double-time Green functions can be found exactly with the help of continued fractions. This immediately yields thermodynamic functions for the spin model considered. The introduced periodic nonuniformity leads to splitting of the magnon band into subbands that, in turns, yields the step-like dependence of the transverse magnetization on the transverse field, the well-pronounced changes in the temperature behaviour of entropy and specific heat etc. All these effects caused by periodic nonuniformity are discussed in detail.

Light scattering in one-dimensional molecular aggregates

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We consider a linear aggregate consisting of N two-level molecules with transition frequency Ω and nearest-neighbour only dipole-dipole coupling J within the frames of pseudospin formalism. In a result we deal with the well-known quantum spin system, spin-$\frac{1}{2}$ XX chain in a transverse field. Light-scattering experiments can be described with the help of the emission spectrum that in the pseudospin formalism can be written as

$$I(\omega) = \sum_{n,m=1}^{N} \int_{-\infty}^{\infty} \mathrm{d}t \mathrm{e}^{i\omega t} \langle s_n^+(t) s_m^-(0) \rangle .$$

We calculate correlation functions of the quantum spin chain obtaining in a result $I(\omega)$. We analyse and discuss the derived frequency shapes at different values of model parameters and temperature.

Nucleation phenomena in atomic fluid in the electrical field

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We have suggested the density functional of grand thermodynamical potential for a fluid of two-level atoms in external electrical field. On the basis of this functional we have studied the appearance of new phases in supersaturated vapour and expanded liquid. We have examined the influence of the field on nucleation and cavitation barriers for that phase transformations and discussed what can be observed in corresponding experimental studies. Some of the presented results were already announced in Refs. [1, 2].

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Critical exponents of the diluted Ising model between dimensions 2 and 4

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We study the ferromagnetic ordering in the diluted Ising model in the region of dilution far from the percolation point. We are interested in the universal characteristics of the critical behaviour of the model with quenched disorder. The calculation are done within the fixed dimension massive field theoretical renormalization group approach, where the asymptotical critical behaviour of the model corresponds to the field Lagrangian with two couplings at ϕ^4-terms of different symmetry.

We obtain the expressions for the β- and γ-functions of the anisotropic mn-vector model in three-loop approximation for general space dimension d. The resulting series of the RG-functions appear to be divergent and we apply resummational procedures in order to extract reliable data on their basis. In particular, special attention is devoted to the effectiveness of different resummation techniques. Finally, the critical exponents for the weakly diluted quenched Ising model ($m = 1$, $n = 0$), as well as estimates for the marginal order parameter component number m_c of the weakly diluted quenched m-vector model are calculated as functions of d in the region $2 \le d < 4$.

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A study of the nematic-isotropic phase transition in liquid crystals by Monte Carlo simulations of lattice models

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A new lattice model of the elongated molecules is proposed to describe the nematic to isotropic (NI) phase transition in liquid crystals. The nearest neighbours interaction via the Berne-Pechukas [1] anisotropic potential is considered. In contrast to widely used Lebwohl-Lasher [2] model an additional parameter of the molecular elongation is introduced.

Monte Carlo simulations of a lattice system of 20^3 molecules are performed. We investigate the temperature behaviour of the internal energy, heat capacity and the scalar order parameter near the NI transition. Particular attention was paid to the influence of the molecular elongation on the transition. The essentially higher values for the latent heat and for the jump of the order parameter at the transition are observed for more elongated molecules, which shows that the NI transition is stronger first order for more elongated molecules [3]. This result is in agreement both with the simulations of hard particles systems near the NI transition and with the simulations of lattice models considered higher order Legendre polynomials in the interaction potential.

The comparison with the experimental data [4] indicate that the behaviour of many real nematics in the vicinity of the NI transition can be described by this model concerning the elongation ratio of molecules from 3 to 5.

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On the description of thermodynamic characteristics of quantum Heisenberg-type cluster systems

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For investigation of critical behaviour of the order-disorder type system containing strongly correlated groups of atoms (clusters) the functional collective variables method is developed. Due to using of recently introduced generalized transition operators [1] (like well-known Hubbard-Stasyuk operators) the compact form of partition function functional is found. Intracluster interactions are described by exchange Heisenberg-type Hamiltonian. The statistic and thermodynamic properties of reference system (non-interacting clusters) are investigated. The method of calculation is developed and the coefficients of non-Gaussian basic distribution of collective variables on generalized transition operators are found.

The critical part of free energy of system is calculated in the frames of layer-by-layer integration method [2]. The recursion relations for the coefficients of block Hamiltonians with dipole-dipole interclusters interactions are found and solved. Due to rigorous treatment of external magnetic field $\vec{h}$ the equation of state is obtained in explicit form. The behaviour of average moment with h and $\tau = \frac{T-T_c}{T_c}$ in the phase transition point neighbourhood is investigated.

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Quantum effects in anharmonic lattice models

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The model of interacting quantum particles performing anharmonic oscillations around their unstable equilibrium positions, which form the d–dimensional simple cubic lattice, is considered. It is shown that the critical point fluctuations of the displacements of particles may be suppressed for all temperatures and in all dimensions if the model is “strongly quantum”. A parameter describing the latter property quantitatively is proposed, it is shown that this parameter infinitely grows when the mass of the particle tends to zero. A sufficient condition for the uniqueness of Gibbs states at given temperature in such a model is established as a restriction of the particle’s mass to be less than a quantity, which may depend on temperature.

The gas-liquid critical point of the binary symmetrical mixture

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The collective variables method with a reference system is applied to the study of the binary symmetrical mixture behaviour in the vicinity of the gas-liquid critical point. The basic density measure (model ρ^4) is constructed in $\rho_{\vec{k}}$- variable phase space which contains the variable ρ_0 connected with the order parameter of the system.

The corrections $\Delta\mathcal{M}_n$ to the basic cumulants in the transition Jacobian arising after integration over unessential collective variables are calculated. It is shown that the problem can be reduced to the calculation of the grand statistical sum functional of 3D Ising model in an external field. The explicit expressions for the critical temperature and critical density are derived and their dependence on microscopic parameters is studied.

Gas-gas equilibrium in binary fluid mixtures

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Microscopic approach to the description of critical phenomena in binary fluid mixtures is proposed. It is based on the method of collective variables with a reference system (I.R. Yukhnovskii, Phase Transitions of the Second Order: Collective Variables Method, World Sci.Publ.Co.Ltd., Singapore 1987; I.R. Yukhnovskii and O.V. Patsahan, J.Stat.Phys., v. 81: 647(1995)). The functional of the grand partition function of the binary mixture is examined in the framework of parameters containing the gas-gas separation point. The physical nature of the relevant order parameter is discussed. The basic density measure is constructed in the collective variable phase space which contains the variable connected with the order parameter of the system. It is shown that the problem can be reduced to the 3D Ising model in an external field. For the symmetrical mixture the explicit expressions for the thermodynamic functions in the vicinity of the gas-gas separation point are obtained.

Description of 3D Ising-like system thermodynamics on the basis of non-Gaussian sixth power measure density

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On the basis of the collective variables method [1], the explicit expressions for the free energy, entropy, internal energy, specific heat and susceptibility as the functions of temperature and microscopic parameters of the system are obtained for the three-dimensional Ising model. The calculations are illustrated by the consideration of simple cubic lattice case and the exponentially decreasing interaction potential. The microscopic parameters are the potential parameters (the radius of effective interaction, the Fourier transform of the potential at zero wave vector value) and the lattice constant. Thermodynamic characteristics of the Ising ferromagnet near the phase transition temperature are determined in the approximation of the non-Gaussian sextic distribution of the spin density oscillation modes (ρ^6 model)[2].

The peculiarity of the microscopic calculation of the expression for the free energy of the system consists in the separation of the contributions from the short- and long-wave modes of the spin moment density fluctuations. The short-wave modes are described by a non-Gaussian measure density and are characterized by the presence of renormalization group symmetry. The calculation of the contribution of the long-wave modes to the free energy is based on the use of the Gaussian measure density as a basic one. Here a direct way of calculation is developed. The results obtained by allowing for the short-wave modes are taken as the initial data. The obtained expression for the free energy in the critical region allows to find other thermodynamic functions of the system.

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Description of the critical behaviour of the lattice systems with n-component order parameter

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The method of calculation of the free energy of the lattice systems with n-component order parameter in three dimensions at the microscopic level is proposed. Mathematical description is produced using method, suggested in [1]. General recursion relations are obtained and the analysis of their approximate solutions in the critical temperature region is performed. Explicit analytical expressions for entropy, internal energy, specific heat, susceptibility near the phase transition point as functions of the temperature are obtained. The dependence of the thermodynamic characteristics of the system and the phase transition temperature on the microscopic parameters of interaction potential is analyzed. As the interaction potential we use an exponentially decreasing function of the distance between the particles situated at the N sites of a simple cubic lattice. Calculations were performed in the framework of the mathematically explicit problem formulation [2]. The equation of state of such systems with n-component order parameter using non-Gaussian measure density is obtained.

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Phase transition of quadrupolar reorientation on magnetodielectrics with tensor interactions

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We study magnetodielectrics with single-ion anisotropy and biquadratic exchange at low temperatures. By means of the local coordinates formalism for systems with tensor interactions, we determine all possible types of uniform ordering.

The transition between quadrupole and quadrupole-angle phases is studied; analytical expression for the temperature of this transition is obtained

$$\theta = \frac{-D\mu}{(\mu-1)\ln[1-\frac{3D}{4K_0(\mu-1)+2D}]}$$

where θ is the absolute temperature, D is the single-ion anisotropy constant, K_0 is the biquadratic exchange constant, and μ is the constant of biquadratic exchange anisotropy.

The $\theta - D$ phase diagram is constructed for different values of μ.

Phase transition in ferroelectrics $Sn_2P_2S_6$ under the high pressure

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The pressure dependences of isothermal volume compressibility for $Sn_2P_2S_6$ ferroelectrics have been investigated in the vicinity of phase transition. The pressure behaviour of critical index was examined as well as the coefficients values were defined in the expansion of thermodynamic potential density in terms of the order parameter power series and their change along the p,T-diagram. Our investigations demonstrated that as we approach to polycritical point (p=0,18 GPa,T=295K) along the phase diagram the coefficients in thermodynamic potential expansion increase occurs. Hence if follows from isothermal volume compressibility along the phase p,T-diagram that with increase in pressure PT for $Sn_2P_2S_6$ crystal drifts apart from a tricritical point, which evidently exists in negative pressures range, approaching to Lifshitz point.

Large supersymmetry breaking for the motion of the electron in a magnetic field

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The motion of electrons in the magnetic field is one of the quantum-mechanical problems, where supersymmetry can be realized as a physical symmetry. It is well known that the $N = 2$ SUSY (supersymmetry) occurs in an arbitrary two-dimensional magnetic field $B_x = B_y = 0$, $B_z = B(x, y)$ and a three-dimensional magnetic field $\mathbf{B}(-\mathbf{r}) = \pm\mathbf{B}(\mathbf{r})$. Recently we have found new classes of three-dimensional magnetic fields in which the motion of the electron possesses the N=2,3,4 SUSY [1]. These are the fields which have some spatial symmetry with respect to the inversion of coordinates.

The question of broken and exact supersymmetry in these fields was studied. Witten introduced an index which can be the criterium of the existence of exact or broken SUSY. It is defined as a difference between bosonic and fermionic ground states with $E = 0$

$$\Delta = {n_B}^{E=0} - {n_F}^{E=0}.$$

If $\Delta \neq 0$ then SUSY must be exact, if $\Delta = 0$ —the question remains opened.

We calculated the Witten index for the Pauli Hamiltonian with the vector potentials mentioned above. The conditions for the vector potentials which lead to exact SUSY in the Pauli Hamiltonian were found. We have also derived the results of Aharonov-Casher theorem about degeneracy of the ground state in the two-dimensional magnetic field by supersymmetric methods.

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Gaussian approximation for Ising model. Variational approach

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It is known [1] that selfconsistent treatment of the order parameter fluctuations in Ising model possess certain difficulties. For instance, such approximations of diagrammatic technique as expansions in the loops order number, summation of the two-tail diagrams for $\langle S\rangle$, $\langle S_1 S_2\rangle$ gives incorrect description of the order of phase transition in the vicinity of the critical point (i. e. first order phase transition instead of the second order one for the three dimensional systems). To solve these difficulty a method of the decomposition of the chain of equations for the spin correlation functions up to the third order was proposed in [2] where it was shown that the proposed decomposition gives correct description of the system behaviour in the vicinity of the critical point.

In this work the variational approach is applied within the functional integrational method. This approach is based on the known Bogoliubov inequality for free energy. In the functional integrational method the hamiltonian is function of the variables $\rho_{\mathbf{k}}(\mathbf{k} \neq 0)$ which describe fluctuations of the order parameter ρ_0. Trial Hamiltonian includes also dependence on the variational parameters $\alpha_{\mathbf{k}}$ which are Fourier-transforms of the effective exchange interaction. Selection of the trial Hamiltonian is performed from the condition that for $\alpha_{\mathbf{k}} \to I_{\mathbf{k}}$ ($I_{\mathbf{k}}$ are Fourier transforms of the exchange interaction) the results equivalent to the one obtained by the summation of the two-tail diagrams are obtained. Finally, a selfconsistent system of four equations is obtained and on its basis it is shown that equation for order parameter gives correct description of the phase transition order.

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Comprehensive investigation of geometric disorder of GaAs surfaces by complementary methods

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This paper presents the results of experimental investigation of the influence of the geometric disorder, one of the most ubiquitous examples of which is surface roughness, on the scattering of the electromagnetic waves within wide spectral region from X-ray to infrared light. Randomly rough (microrelief) surfaces prepared with wet chemical anisotropic etching have been used because they have the certain geometric disorder without having damaged subsurface layers and even the improved electronic properties. The X-ray grazing incidence reflectivity, optical specular reflection and profilometry are used for characterization of the surface roughness. The optical and profilometry measurements relate to the macrorelief of the surface which defines a type of a surface (Gaussian, exponential or fractal one). The X-ray specular grazing scattering measurements compared with the computer simulations based on Fresnel theory give average micro-roughness. The influence of micro- and macro-irregularities on data of both Raman scattering and surface phonon spectroscopy are studied. The existence of Raman scattering lines from LO- and TO-optical phonon modes, their spectral position and the additional broadening observed are caused mainly by geometric disorder of the surface. These results are compared with both the dispersion and the damping of surface phonon polaritons excited by attenuated total reflection (ATR) method. The crystal structure perfection of anisotropically etched GaAs surfaces are confirmed by complementary methods based on the electromagnetic waves scattering. An anomalous small damping of surface modes on the some microrelief of GaAs have been observed by both ATR and Raman scattering methods.

Temperature-induced metal-insulator transition in a narrow-band model with non-equivalent Hubbard sub-bands at half-filling

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In present paper metal-insulator transition is studied in the model of narrow-band material with non-equivalent Hubbard sub-bands. The model is defined by intra-atomic Coulomb repulsion U and hopping integrals t, $\tilde{t}$, t'; t, $\tilde{t}$ describe "translational" hoppings of holes and doublons respectively, t' describes a process of paired creation and annihilation of holes and doublons. A distinction of these hopping integrals is caused by taking into account of correlated hopping of electrons.

Quasiparticle energy spectrum is computed with the help of Green function method using a generalized mean-field approximation [1]. With the help of electron energy spectrum we obtain the energy gap width ΔE as the function of the concentration of polar states c (holes or doublons), the half-width of hole band w, the half-width of doublon band $\tilde{w}$, hopping integral t', the number of nearest neighbours to a site z, intra-atomic Coulomb repulsion U

$$\Delta E = -(1-2c)(w+\tilde{w}) + \frac{1}{2}(Q_1+Q_2),$$
$$Q_1 = \sqrt{[B(w-\tilde{w})-U]^2 + (4czt')^2},$$
$$Q_2 = \sqrt{[B(w-\tilde{w})+U]^2 + (4czt')^2}, \quad B = 1-2c+4c^2.$$

Concentration-dependence of energy gap leads to the fact that with increase of temperature the energy gap width is decreased. Thus narrow-band system can turn from a metallic state into an insulating state with increase of temperature.

For some values of U and w_0 (w_0 is half-width of band without taking into account of correlated hopping of electrons) we find the values of temperature when narrow-band material turns from a metallic state into an insulating state. We show that at given U/w_0 metal-insulator transition in model with non-equivalent Hubbard sub-bands can take place at smaller temperature than in the Hubbard model. It testifies on the fact that taking into account of correlated hopping is important for a consideration of metal-insulator transition problem.

The obtained results are applied to the interpretation of the experimental data.

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Mott-Hubbard transition in a model with a doubly degenerated band

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In present paper the method developed in [1] for the Hubbard model is generalized with taking into account of twofold orbital degeneration which is characteristic for transition metal disulphides. The microscopic model is constructed to describe the electron subsystem of magnetic (ferromagnetic in saturated magnetic state, paramagnetic) with narrow energy bands.

The quasiparticle energy spectrum which allows to study initiated by external influences metal-insulator transition is calculated. We obtain the chemical potential, concentration of current carriers and energy gap width as a functions of model parameters and temperature. In the case of strong Hund's-rule coupling ($U \gg U-J$, $U \gg t$, where U is the intra-atomic Coulomb repulsion, J is the intra-atomic exchange energy, t is the electron hopping integral) the energy gap width is

$$\Delta E = -2w(0.75-1.5c) + \frac{1}{2}\left\{[(U-J)+0.5w)]^2 + 8c^2w^2\right\}^{1/2} + \\ + \frac{1}{2}\left\{[(U-J)-0.5w]^2 + 8c^2w^2\right\}^{1/2}.$$

where c is the hole concentration, $2w$ is the bandwidth without taking into account of the correlation effects.

The conditions of metallic and insulating states are determined. The obtained results allow to interpretate the observing peculiarities of physical properties of narrow-band materials and to predict the changes of such properties under the action of external influences (pressure, temperature, magnetic field, photoeffect). In particular, this model allows to explain metal-insulator transition which is observed in NiS_2, $(V_{1-x}Cr_x)_2O_3$.

Specific narrow-band effects and possibilities of its observation and application are discussed.

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The semiconductor microcrystals embedded in solid matrices of the natural zeolite

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The paper deals with the problems of creating and investigating new materials on the base substitutive solid solutions of the semiconductor crystals incorporated into zeolite matrix. $In_xTl_{1-x}I$ ($0.2 < x < 0.95$) semiconducting substitutive solid solutions and $Na_8[Al_8Si_{40}O_{96}]\div 24H_2O$ zeolite of the mordenite type (Na-MOR) in the matrice role have been used. The method of preparing the $In_xTl_{1-x}I$ clusters is based on the thermovacuum processing. The one-dimensional emptiness of Na-MOR is little bit smaller than NaX or NaY synthetic zeolite. However, the higher characteristic energy compensates a few little bulk of the micropores. Na-MOR samples were powdered finely and dehydrated in vacuum. It is determined that Na-MOR gives back about 10% of water at the temperature $363 \div 633$ K and the all water at the $823 \div 873$ K during 3-6 hours without crushing of the space structure of the zeolite framework. $In_xTl_{1-x}I$ molecules were incorporated into the zeolite supercages by physical absorption. Optimal temperature regime is within $653 \div 713$ K respectively to In/Tl ratio. The absorption infrared spectra and luminescent spectra of the pure Na-MOR-matrices are investigated. A few models are proposed for $In_xTl_{1-x}I$ microcrystals embedded in zeolite solid matrice.

Theory of X-ray (neutron) diffuse scattering from binary alloys

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As is well known a knowledge of atomic static displacement (ASD) amplitudes and the short-range order (SRO) parameters is required to calculate the diffuse scattering intensity theoretically. The problem, "reverse" to the stated above, has been solved ordinary: the SRO parameters are searched on the basis of experimental data on the X-ray diffuse scattering intensity and values of the ASD amplitudes, determined phenomenologically. It means that the ASD and the binary correlation function Fourier components are treated as independent parameters of a theory.

A microscopic approach to calculate the X-ray diffuse scattering intensity from disordered binary alloys is advanced in the paper given. It is a feature of the approach proposed that:

1. The ASD and the SRO effects are considered within the same collective variables method [1] and their mutual influence on each other is investigated for the first time.
2. The explicit expression for the Debye-Waller factor, which contains thermal and static terms, is obtained.

Equation for the X-ray (neutron) diffuse scattering intensity $I(q)$ is derived and analysed. Original moments of the theory are emphasized. Theoretical results are illustrated by $I(q)$ calculations performed for disordered alloys of $K-Cs$ and $Ca-Ba$ systems. It is shown that the SRO and the ASD contributions to the $I(q)$ could not be treated separately. The ASD has drastic effect on the binary correlation function Fourier transform behaviour in the Brillouin zone. Dependence of $I(q)$ on temperature and alloy concentration is investigated.

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Model calculation of the influence of the nonhomogeneous semiconductor surface layer on the reflection and phase spectra in the resonance region

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The presented work contains the theoretical analysis and model calculation of the effect of the surface state on the amplitude and phase spectra forming in the resonant dispersion region of the dielectric function, which is strong, especially in wide bandgap semiconductors due to their large exciton radius and oscillator strengths. The model calculations of the reflection spectra are based on the non-resonance layer at the semiconductor surface. Data analysis shows that:

1. The spectral position of the reflection minimum oscillates in the range of the longitudinal-transverse splitting of energy E_{lt} when the thickness d of the surface layer and damping factor γ are changed.
2. If the hodograph of the reflection complex amplitude $\tilde{r}$ passes through its common reference point, the phase spectra changes as "S"$\longleftrightarrow$"N" independently from the nature of dispersion $\tilde{\varepsilon}(\omega)$. "S" type of phase contour was observed in the range $\rho_{12} < \rho_{23}$, where indexes 12 and 23 correspond to the vacuum-layer and the layer-bulk crystal interfaces $r_{ij} = \rho_{ij} \exp(i\varphi_{ij})$. When the condition $\rho_{12} > \rho_{23}$ is satisfied then the phase spectra have the "N" type form.
3. It is suggested that multy-oscillations of the reflection spectra change when the resonance frequency changes in the near-surface region.

Magnetic properties of dilute alloys: equations for magnetization and its structural fluctuations

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The dilute Heisenberg ferromagnet is studied taking into account fluctuations of magnetization caused by disorder. A self–consistent system of equations for magnetization and its mean quadratic fluctuations is derived within the configurationally averaged two–time temperature Green's function method. This system of equations is analysed at low concentration of non–magnetic impurities. Mean relative quadratic fluctuations of magnetization are revealed to be proportional to the square of concentration of impurities.

External pressure effects in deuterated crystals of KH_2PO_4 family

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We propose a unified approach to the description of deformed by the non-lowering the crystals symmetry pressures – hydrostatic and uniaxial $p = -\sigma_3$ – state of deuterated ferroelectrics and antiferroelectrics of KH_2PO_4 family. The calculations are performed in the framework of the proton ordering model, using the four-particle cluster approximation for the short-range deuteron correlations and the mean field approximation for the long range interactions. Within the Glauber approach, the relaxational dynamics of the crystals is considered in the approximation of the time-independent strains. A fair agreement with the available experimental data for the pressure dependences of the transition temperature and static dielectric characteristics of the MeD_2XO_4 (Me = K, Rb, ND_4, X = P, As) crystals is obtained. Possible pressure dependences of other characteristics of these crystals are stated, if those have not been studied experimentally yet. The crucial role of the pressure changes in the hydrogen bond geometry (the D-site distances) in the pressure dependences of the transition temperature and dielectric response of these crystals is shown. Effects of hydrostatic and uniaxial pressures are compared, and the possible changes in the D-site distances with the uniaxial pressure are discussed. Some peculiarities of dipole moment formation in the hydrogen bonded crystals are elucidated.

Influence of hydrostatic and uniaxial σ_3 pressures on phase transition and dielectric properties of KH_2PO_4 type ferroelectrics and $NH_4H_2PO_4$ type antiferroelectrics

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On the basis of the proposed earlier model [1], we study the influence of hydrostatic and uniaxial $p = -\sigma_3$ pressure on the phase transition and dielectric properties of KH_2PO_4 type ferroelectrics and $NH_4H_2PO_4$ type antiferroelectrics. In the four-particle cluster approximation, the free energies, thermodynamic potentials, and specific heats of these crystals are calculated; the equation for the order parameter and lattice strains is obtained, and the equation for the transition temperature is found. For the first time, the components of the dielectric permittivities of KH_2PO_4 type ferroelectrics and $NH_4H_2PO_4$ type antiferroelectrics are calculated. Variation of the tunnelling integral of a proton, moving in the double Morse potential, with the hydrostatic pressure is studied, taking into account the experimental linear pressure dependences of the H-bond length and the H-site distance.

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Influence of uniaxial stress $\sigma_1 - \sigma_2$ on phase transition, thermodynamic and dynamic properties of deuterated ferroelectric orthophosphates

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We propose an approach for the description of the uniaxial stress influence $\sigma_1 - \sigma_2$ on hydrogen bonded ferroelectrics and antiferroelectrics of KH_2PO_4 family. In the four-particle cluster approximation, we calculate the free energy, thermodynamic potential, thermodynamic and dynamic characteristics of the crystals as functions of external stress and temperature. A thorough numerical analysis of the uniaxial stress influence on the phase transitions in KD_2PO_4 and $ND_4D_2PO_4$ crystals is performed. The pressure induced phase transitions are studied.

Correlated effective field approximation for Ising model with arbitrary interaction

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Correlated effective field approximations are widely used in the theory of Ising systems with the nearest neighbour interaction [1,2]. On the basis of the approximate solution of the Callen identity

$$\langle S_k \rangle = \langle \tanh(\beta \sum_{i \neq k} J(R_i - R_k) S_i + \beta h_k) \rangle$$

these methods give quite satisfactory results not only for the most thermodynamic functions but also for the inelastic neutron scattering cross section [3]. We apply the correlated effective field approximation proposed in Ref.1 to the model with arbitrary interaction. We analyze the thermodynamic functions of the model with different interactions and study the caused by the long range character of the interaction finite line width of the inelastic neutron scattering cross section.

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Dynamics and thermodynamics of pseudospin models. Two-particle cluster approximation

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For quantum pseudospin models, the consistent formulation of the cluster expansion method is proposed for the first time. This method allows one to obtain the Ornstein-Zernike type equation for the temperature cumulant Green functions of any order. In the two-particle cluster approximation, an explicit expression is obtained for the pair cumulant Green function. In the random phase approximation, we calculate and study the free energy, entropy, specific heat, longitudinal susceptibility, static correlation functions $\langle S_n^x S_0^x \rangle$ and $\langle S_n^z S_0^z \rangle$, and spectra of elementary excitations and their integral intensities for the quasi-one-dimensional Ising model in transverse field. We show, that in the vicinity of the transition point, an essential suppression of the soft mode by the short-range correlations takes place. The obtained results are used for description of experimental data for quasi-one-dimensional ferroelectrics with hydrogen bonds.

Van Hove singularity and D-wave pairing in disordered superconductors

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We apply the coherent potential approximation (CPA) to a simple model for disordered superconductors with d-wave pairing and demonstrate that whilst the effectiveness of an electronic Van Hove singularity to enhance the transition temperature T_c is reduced by disorder it is not eliminated. In fact we give a qualitative account of changes in the T_c vs. doping curve with increasing disorder and compare our results with experiments on the $Y_{0.8}Ca_{0.2}Ba_2(Cu_{1-c}Zn_c)_3O_{7-\delta}$ alloys.

AC magnetic susceptibility of the granular Hg-containing HTSC

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Results of the experimental and calculated from the critical state models temperature and fields dependences of the dynamical magnetic susceptibility $\chi_n = \chi_n' - i\chi_n''$ for the Hg-containing HTSC-samples are discussed.

Samples of Hg-1212 and Hg-1223 with the nominal contents $Hg_{0.8}Pb_{0.2}Ba_2Ca_1Cu_2O_{6+\delta}$ and $Hg_{0.8}Pb_{0.2}Ba_2Ca_2Cu_3O_{8+\delta}$, respectively, are prepared using the solid/vapour phase reaction with the use of Hg-source [1].

Measuring of the χ_n' and χ_n'' are carried out using the inductive Khartshorne bridge with the direct writing down of the uptake signal by computer and the following programme processing of the gathered data.

Applying such methodics gave us the possibility to simplify distinguishing process of the in-phase χ' and quadratic χ'' components and simultaneously to receive the information about the behaviour of some magnetic susceptibility harmonics. Critical state model [2] and modified one [3] were used for the calculation of the theoretical dependences of the magnetic susceptibility versus temperature. Critical parameters H_{c1j}, H_{c2j} and f_n obtained from the field dependences of the magnetic susceptibility have been used for the calculations. Parameters which were closer defined are London depth penetration λ_g, pinning forces $\alpha_j(0)$ and $\alpha_g(0)$. Initial means $\lambda_g(0)$ have been obtained as overall $\lambda_g^{ab}(0)$ and $\lambda_g^c(0)$ (4). The best coordination with the experiment have been obtained for the quadratic dependence α_j versus T ($\alpha_j \sim (1 - T/T_c)^2$) what means the formation of the SNS links between granules.

Parameters of the critical state are shown in the table and they have been obtained from the comparing of the experimental data and the model.

Compound	$\langle R_g \rangle$ μm	$\langle \lambda_g \rangle$ μm	$\alpha_j(0)$ ATm^{-2}	$\alpha_g(0)$ ATm^{-2}	$j_{cj}(0)$ Amm^{-2}	$j_{cg}(0)$ Amm^{-2}	Link type
(Hg,Pb)-1212	10	0.4	$1.3 \cdot 10^4$	$1.1 \cdot 10^7$	$5.2 \cdot 10^3$	$8.5 \cdot 10^6$	SNS
(Hg,Pb)-1223	10	0.3	$1.79 \cdot 10^3$	$1.78 \cdot 10^7$	$3.2\dot{1}0^2$	$1.4 \cdot 10^7$	SNS

Table 1. Parameters of Hg-containing samples closer defined corresponding to the models.

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Extra oxygen and carrier distribution in CuO_2 layers in $HgBa_2Ca_{n-1}Cu_nO_{2n+2+\delta}$ compounds (n=1,2,4)

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The numerous investigations have shown, that in high-T_c La-, Y-, Bi-, Tl-based compounds the electrostatic interactions is the key factor in the charge distribution between the CuO_2 layers. The determination of the equilibrium state of the crystal lattice by minimization of the total energy E_{tot} is proposed to elucidate role of the electrostatic interactions in Hg-HTCS. E_{tot} contains the electrostatic (Madelung) and band energy E_b [1]. The approximation of non-interacting holes (U=0, where U is parameter of Coulomb repulsion on the same site) is used to evaluate E_b. The intralayer transfer integral was defined within the framework of the Cyrot's model [2]. Finally the following expression was obtained for E_b:

$$E_b = \frac{\pi T_c}{\delta} \sum_i p_{hi}^2,$$

where T_c is the superconducting critical temperature, δ is the number of holes, p_{hi} is the charge carrier density of the i-th CuO_2 layer. We assume that the holes distribute between the CuO2 layers uniformly for compounds with n=2. The inequivalency of the inner and outer layers is accounted for n=4. The minimization of total energy was performed with respect to contents of extra oxygen. The structure data of the series of the samples with different contents of the extra oxygen is used for the analysis [3]. The parameter which determine the distribution of holes between Cu and O sites during the calculation was selected to coincide δ_{min} and experimental data for one sample of the series. The calculations for the other samples satisfactory describe the changes of δ and indicate the prefered localization of the holes on the oxygen site according to the data for other classes of HTSC.

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The dependence of ferromagnetic ordering temperature of many-component amorphous magnets on the concentration

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The many component amorphous magnetic atoms system with Heisenberg exchange interaction was investigated with the help of functional integral approach. The magnetic part of the free energy for this system was obtained within random phase approximation (RPA). Using the expansion of the free energy in powers of order parameter, the Curie temperature of two-component amorphous ferromagnet is found taking into account the topological disorder and magnetic fluctuations. The explicit expression for the ferromagnetic ordering temperature as a function of concentration of magnetic atoms was calculated. When the atoms are considered to be hard spheres with the liquid-type disorder, the numerical calculations of the concentration dependence of the Curie temperature for two-sort amorphous magnets showed that there exists the critical concentration x_c of one of magnetic components ($T_c(x_c) = 0$) (it corresponds to decrease of effective radius of exchange interaction in the model exchange integral).

The dependence of concentration of nonmagnetic atoms on the expression of Curie temperature of many-component magnetic amorphous system is also obtained and discussed.

Mechanism of forming of the electret state of porous silicon by hydrogen defects

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The perspective of porous silicon application for dielectric electronics and optoelectronics is connected with unsufficient stability of electrical and light emitting properties at different temperatures that may be conditioned with electrical activity ions drift in this material.

In this connection we have consider our aim to investigate thermoelectret condition of porous silicon. For this research we have used the thermostimulated discharge currents (TSDC) analysis, which ordinary is applied for electrets studying.

The heterostructures — porous silicon-silicon substrate at first was polarised at 177-450K and voltage 100V for obtaining of TSDC spectrum. Samples were isolated from copper electrodes with thin dielectric films. Thermostimulated polarisation was conducted by linear with time heating and cooling applying of the constant electrical field to specimen. Specimen was linear heated at 195K - 520K for obtaining TDSC condition. Values of depolarisation current about 10^{-13}A were measured in this process. The dependence of TSD current from temperature had some peaks, which we classified into two bands at 300–425K and 450–525K temperatures. We have obtained energy distribution function of ions and their activation energy according to experimental dependence TDS current from temperature. For that we have solved numerically Fredholm's integral equation, that described TSDC process in disordered structures. Our calculations witness about existence of the two types of ionised defects in PS with activation energies near 0.8 and 1.0 eV.

We have explained existence of TSDC phenomena in porous silicon and experimental character of TSDC spectra: on the surfaces of porous silicon the thin natural film of amorphous SiO_xC_y, exists, and covers huge area of pores. These films may be responsible for dielectric properties of porous silicon. Separately, for amorphous SIO_x TSDC band at 360–410K temperatures was explained by H^+ ions migration in SiO_x and second band at 450-525K temperatures was explained by alkali ions migration. So electret state of porous silicon exist due hydrogen defects and alkali ions migration on the surface of porous silicon.

Raman scattering in crystals with order-disorder type phase-transitions

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A microscopic approach to the description of phonon and electron Raman scattering in the dielectric crystals with order-disorder type phase transitions is developed. The theory is based on the "operator" two-time Green functions formalism which is applied for the construction of the polarizability operators entering the general expression for the effective cross-section of Raman scattering. An equations of motion method and a perturbation series expansion over the electron and phonon variables are used. In the case of crystals with ordering structure units the procedure of averaging over their various configurations is elaborated.

The developed microscopic scheme is applied to the investigation of the Raman scattering in the ferroelectrics with hydrogen bonds and in the crystals with the structural phase transitions of Jahn-Teller type accompanied by the ordering of localized electron quadrupole momenta. The problems of the configurational splitting in spectra of scattering on the internal vibrations of ionic groups as well as of the additional (caused by the redistribution of mean occupancies of the low lying energy levels) temperature dependences of the electron and phonon Raman lines intensities are investigated more detailly.

The ferroelectrics of KDP family and the crystals with structural phase transitions of RXO_4–type (R are rare-earth ions) are taken as an object of study. The possibilities of direct experimental manifestation of the considered effects are discussed.

Polarizability operator and Raman scattering intensity for systems with Hubbard interaction

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The aim of this investigation is to study nonphonon contributions to Raman light scattering in the systems with the Hubbard type interaction between electrons. This problem remains a subject of interest in spite of the success achieved in the description of the magnetic or electron Raman scattering as well as in the investigation of more complicated scattering mechanisms in the cases of partial filling of electron bands (P.Fleury, R.Loudon, 1968; B.S.Shastry, B.I.Shraiman, 1990).

We start from the general expression for the Raman scattering tensor in terms of the time correlation function calculated on polarizability operators

$$\hat{P}^{\beta\alpha}_{\vec{k}'\vec{k}}(\omega,t) = -\int\limits_{-\infty}^{+\infty} ds\; e^{i\omega(t-s)} \left\{\left\{\hat{M}^{\beta}(\vec{k}',t)|\hat{M}^{\alpha}(\vec{k},s)\right\}\right\}$$

($\hat{M}^{\alpha}(\vec{k})$ is a dipole momentum operator of a crystal in the $\vec{k}$–representation). To construct the $\hat{P}$ operator, the equation of motion method for "unaveraged Green functions" $\{\{A(t)|B(t')\}\} = -i\Theta(t-t')\,[A(t),B(t')]$ is used (I.V.Stasyuk, Ya.L.Ivankiv, 1987). The solutions of these equations are built in the form of operator series.

This approach is applied to the cases of the Hubbard and the $t-J$ models when the caused by interaction with light dipole transitions into the upper Hubbard subband as well as into situated at higher energies electron states are taken into account. The electron transfer parameter $t_{i,j}$ and the effective exchange constant J_{eff} are used as formal expansion parameters at the construction of the $\hat{P}$ operator. The expressions for the Raman scattering tensor in terms of the correlation functions calculated on the Hubbard operators are obtained. For the case of the $t-J$ model the possibility of the description of deviations from the pure magnon scattering at the some hole doping level is analysed.

Thermodynamics of system with strong short–range electron correlations in generalized random–phase approximation

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The generalized random phase approximation (GRPA) was proposed recently as a method of investigation of pair spin and charge correlations in systems with strong short–range Hubbard interaction. Due to the inclusion of interaction terms into zero–order Hamiltonian the diagrammatic technique for Hubbard operators was used. On this basis for the Hubbard model with local anharmonicity (pseudospin–electron model) the dielectric response function was investigated [1]. It was found that there are the regions of model parameters where dielectric instability and instability with respect to the charge separation take place but the problem of evaluation of thermodynamic functions in this approximation remained unsolved.

In this work the self–consistent generalization of GRPA scheme which allows to calculate thermodynamical potential and other characteristics of models with strong short–range electron interaction is proposed. Firstly, all diagrams with one–tailed loop–like inclusions into one–site cumulants are summarized what corresponds to the extended mean field approximation. Secondary, the additional renormalization of electron Green functions due to the shifts of energy levels as well as renormalization of their end parts are performed. The constructed within this approach loop–like diagrams are taken into account at the calculation of thermodynamical potential.

This approach is used for the investigation of thermodynamical properties of the two–sublattice Hubbard model with described by pseudospins local anharmonicity. The influence of electron subsystem on the possible ordering of pseudospins is studied. The phase diagrams of the model are built. The anomalies in the temperature and local field asymmetry dependence of dielectric susceptibility of the system are investigated. The obtained results are applied for the description of the anharmonic apex oxygen subsystem behaviour in the layered high–T_c superconductors.

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Pseudospin–electron model of high-T_c superconductors in large dimensions

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Energy spectrum and thermodynamics of the pseudospin–electron model introduced at the consideration of the anharmonicity effects in high–T_c superconductors are investigated in the dynamical mean field approximation developed for the description of the strongly correlated electron systems in the limit of infinite space dimension $d = \infty$. In the limit of zero electron correlation $U \to 0$ this model is analytically exactly soluble within this approach: in the $\mu =$ const regime the first order phase transition with the jump of the pseudospin mean value $\langle S^z \rangle$ and reconstruction of the electron spectrum can realize, while in the $n =$ const regime the phase separation in electron subsystem can take place for certain values of the model parameters.

On the basis of the obtained results the applicability of the approximate schemes previously used for the investigation of the pseudospin–electron model are discussed.

Phase transitions in pseudospin-electron model with direct interaction of pseudospins

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Pseudospin–electron model is one of the basic models for consideration of phenomena caused by anharmonic structure components in high-T_c superconductors. The model is also used for the description of proton-electron interactions in crystals with hydrogen bonds. If the direct pseudospin interaction $-\sum_{ij} J_{ij} S_i^z S_j^z$ is taken into consideration the pseudospin part of the Hamiltonian of the model has the form of Ising's Hamiltonian in the external field $-h\sum_i S_i^z$. The electron part corresponds to the Hubbard model. The coupling between two subsystems is given by contact interaction $\sum_{i\sigma} n_{i\sigma} S_i^z$.

The analysis of thermodynamic properties of the model in the case of zero electron transfer is performed. The interaction J_{ij} is assumed to be of ferroelectric type and is taken into account in the mean field approximation. At the exact treatment of the pseudospin-electron interaction the thermodynamic potential Ω and free energy F are derived. A set of equations based on the equilibrium conditions in the regimes $n = const$ and $\mu = const$ are written for the order parameter $\eta = \langle S^z \rangle$ and chemical potential μ. The solution of the mentioned set of equations is performed using numerical methods. The dependencies of $\eta(h)$, $\Omega(h)$ and $F(h)$ for various values of n(or μ), T, g and J were analyzed. The analytic analysis for the limit case of $T = 0$ was performed.

It is shown that the interaction with electrons leads to the splitting of the transition in Ising model into two or three (depending on the value of U) phase transitions taking place at different values of h. The first order phase transitions at the change of temperature with a jump-like behaviour of $\langle S^z \rangle$ are possible. The phase diagrams $(U, h; T = 0)$, $(n, h; T = 0)$ and (T, h) are built. In addition to phases which correspond to $\eta(T = 0) = \pm\frac{1}{2}$ the phases with intermediate values $\eta(T = 0) = \frac{1}{2} - n$, $\frac{1-n}{2}$ and $\frac{3}{2} - n$ appear. The $\mu(n)$ dependencies at various values of the model parameters are investigated. The instability of phases with intermediate values of η with respect to phase separation is established.

The interpretation of the anomalies of thermodynamic characteristics which have been found in the case of nonzero electron transfer is given.

Vacancy induced rearrangement phase transitions in apex oxygen subsystem of HTSC with YBaCuO-type structure

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Thermodynamics of apex oxygen rearrangement processes in the $YBa_2Cu_3O_{7-x}$ high–T_c superconductors affected by oxygen vacancies in CuO chains is studied in the framework of Mitsui model where two possible localizations of an apex oxygen are described by the pseudospin formalism. The influence of vacancies is modelled by the acting on the pseudospins longitudinal bimodal random field (with values h and h_{vac}) for both cases of nonequilibrium and equilibrium vacancy distributions. Thermodynamic functions of the model are calculated in the mean field approximation for long–range interactions with an exact treatment of the intracell interaction of pseudospins which belong to different sublattices.

The system can have various possible phases which correspond to possible arrangements of apex oxygens in different sublattices: nonequivalent nonpolar phases with the preferably antiphase localization and the polar phase with the partially synphase one. Results of calculations show that for the strong enough negative value of the intracell interaction parameter j or for the intercell interaction parameter $a < -1$ the polar phase is suppressed and the direct phase transition between nonpolar phases is possible (bistable behaviour). The dielectric susceptibility has an abrupt jump in the region of this phase transition.

For certain values of the system parameters there are three nonequivalent nonpolar phases in the low–temperature region which transform one to another at the variation of the vacancy concentration. In the case of the equilibrium vacancy distribution the intermediate phase could become unstable with respect to a phase separation.

Influence of an external pressure on the system is investigated in the conjecture that it leads only to the change of the asymmetry fields h and h_{vac}. Increase of the pressure has the effect similar to increase of the concentration but there is only one phase transition region at the pressure variation.

Orientational-tunneling kinetics of proton transport along the hydrogen-bonded chains

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Various kinds of physical and biological objects contain the hydrogen-bonded molecular systems in which the hydrogen bonds network plays a dominant role in their properties. In particular, the theoretical and experimental investigations of the proton mobility in water, proteins, at the surfaces and inside of the solid-state materials have received much attention recently.

In this work the problem of proton dynamics along the hydrogen-bonded chains is considered. The proton transport process is described in the frame of the Grotthuss mechanism which involves the proton movement within the hydrogen bond with the further interbond hopping caused by librational "tumbling" of the neighbouring ionic group. The latter effect leads to the appearance of the so-called Bjerrum defects. The mobility of these defects of D- and L-type determines the protonic conductivity coefficients. On this basis the theoretical model is proposed which includes additionally the interaction between protons and the vibrational modes of the ionic groups that results in the strong polaronic effect.

Protonic conductivity and diffusion are studied in the frame of Kubo linear response theory. The temperature and frequency dependence of the kinetic coefficients is evaluated numerically. The influence of the strong intrabond proton coupling ad well as the polaronic effect on the proton transport is analysed additionally.

Influence of the square-root Van Hove singularity on the critical temperature of high-temperature superconductors

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It is shown that the square-root Van Hove singularity in the density of states $\nu(E_F) \sim (E_F - E_0)^{-1/2}$, associated with the extended saddle-point features (ESPF) in the electron spectra of the cuprate metal-oxide compounds with hole-type conductivity [1,2], leads to the nonmonotonic dependence of the critical temperature T_c of the superconducting transition on the concentration n_h of the doped holes. The effect of the square-root singularities on superconducting properties was considered earlier in [3,4] with the weak coupling approximation, giving a finite (and close to maximal) value of T_c for sufficiently high values of n_h, when the Fermi level E_F touches the bottom of the saddle E_0 in the energy spectrum. Such an approach however is unapplicable in this limit as the coupling constant $\lambda \sim \nu(E_F)$ diverges with the density of states. In the present report the concentrational dependence of the critical temperature is investigated in the strong coupling approximation. The account of the strong coupling effects leads to the renormalization of the coupling constant $\widetilde{\lambda} = \lambda/(1+\lambda)$ resulting in cancellation of the square-root divergency and, eventually, in the linear dependence of $T_c \sim (E_F - E_0)$ on the Fermi energy on ESPF, i.e. T_c approaches zero in the limit $E_F \to E_0$. The ensuing concentrational dependence of T_c agrees qualitatively with the experimental data for the overdoped cuprates.

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Two-ray laser spectroscopy of deep local centers in $ZnSiP_2$

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The experimental optical method for determination of band structure and energy of local centers is developed. The method is based on using of two laser rays - one with high intensity and small intensity probe ray. In the paper this method has been applied for $ZnSiP_2$ single crystals grown from tin. $ZnSiP_2$ crystals have the structure of halcopyrit and hole type of conductivity. Measurements were taken at 293K by above-mentioned laser amplitude - modulated spectroscopy method. We have carried out the analysis of relaxation kinetics of occupancy density of deep dopant centers at high and at low levels of generations electrons and holes in bands by laser impulse. The impulse neodime laser (15 nsec) and impulse xenon lamp (150 nsec) have been used as modulating source and as probe source, respectively. These two sources were synchronized.Three types of deep levels 0,P and R have been discovered. The photoionization cross-sections for the electron transitions from O or P centers into c-band are obtained - $0.6 \times 10^{-17} cm^2$ and $1.3 \times 10^{-17} cm^2$, respectively. The energy diagram of deep levels of impurity origin and the scheme of optical and recombination transitions have been built.

The influence of heterointerface onto band gap value of epitaxial structures $Ga_xIn_{1-x}As_yP_{1-x}/InP$

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The heterointerface in low-dimensional structures with a large lattice constant mismatch ($f = \Delta a/a \geq 2\%$) should significantly change the band structure and main characteristics of pseudomorphical low-dimensional systems. The aim of this communication is to propose the method for estimating of heterointerface strain influence in quaternary solid solution $Ga_xIn_{1-x}As_yP_{1-x}/InP$ on the band gap value. The method is based on the model of deformation mismatch on the heterointerface is accommodated by planar elastic deformation.

For investigated heterostructure the deformation dependence of band gap can be expressed an follows:

$$\widetilde{E}g \approx Eg(0) + \frac{5}{4}\left[S_\perp - S_\parallel \frac{C_{11}+2C_{12}+4C_{44}}{3(C_{11}+2C_{12})}\right]\varepsilon_\perp, \qquad (1)$$

where $Eg(0)$ is a bandgap value without deformation, $S_\perp$ is a constant of deformation potential normally to the heterointerface plane, $S_\parallel$ is a deformation potential constant parallel to the heterointerface, C_{ij} are the elasticity modules of solid solution, $\varepsilon_\perp$ is a deformation tensor normally to the heterointerface plane. The dependence of $\varepsilon_\perp$ from molar parts x and y is

$$\varepsilon_\perp = \frac{1}{a_{InP}}\frac{3(C_{11}+2C_{12})}{C_{11}+2C_{12}+4C_{44}}\left[a_{GaAs}xy + a_{InAs}(1-x)y + \right. \qquad (2)$$
$$\left. + a_{GaP}x(1-y) + a_{InP}(1-x)(1-y) - a_{InP}\right].$$

The estimation of Eg_1 (1) accounting (2) in dependence of solid solution composition x, y correlates with experimental results [1]. Besides that we have estimated the coefficient $\frac{d\widetilde{E}g}{\partial\sigma}$ of epitaxial structure based on expressions (1), (2) and $\sigma = -2C_{44}\varepsilon_\perp$.

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Radiation induced effects in ternary amorphous chalcogenides

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A new experimental results concerning optical studies of radiation–induced effects in vitreous chalcogenide semiconductors (VChS) at the range of fundamental absorbtion edge are discussed. The ternary systems of VChS, such as As-S-Sb, As-S-Ge, As-S-Tl, As-Se-Sb, As-Se-Ge, Sb-S-Ge, have been investigated over a wide range of compositions including ones with topological phase transitions, structural and chemical transitions, as well as nontransitional quasibinary substitutions. All investigated samples have been prepared by direct synthesis in evacuated quartz ampoules using high purity initial components. They have been irradiated by gamma–quanta with 1,25 MeV average energy at the power of exposure doses over 20 Gy/sec. It is obtained that radiation treatment leads to the long–wave shift of the fundamental absorption edge for VChS samples. These radiation–induced changes of absorption spectra are unstable. They restore to some residual value after the period of 2–3 months. The other way to partial restoration of the radiation–induced spectra is thermal annealing at the temperatures just below softening point Tg. It testifies to the existence of two components of this effect: statical and dynamical ones. Above mentioned results are recalculated in the form of spectral dependences of the absorption coefficients difference (before and after gamma-irradiation). This curve for each VChS sample has a well expressed maximum, which shifts to the low-energy part of spectra with increasing of average coordination number. Compositional–, time– and temperature–related dependences of these radiation–induced changes are studied. Obtained results are explained in a framework of the model of coordination defects formation in the VChS structural network.

The baric changes of optical properties of KDP crystals

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Influence of the uniaxial mechanical pressure σ_m (m=1,2,3) on the temperature (77-300K) and spectral (400-700nm) dependence of the birefringence Δn_i and phase transition (PT) temperature T_c of KDP and DKDP crystals is investigated.

In paraphase of KDP and DKDP crystals uniaxial pressures σ_3 and σ_1 leads to the increase and to the decrease of Δn_2, respectively, and $|\delta\Delta n_2(\sigma_1)| > |\delta\Delta n_2(\sigma_3)|$. The sample compression does not practically influence its dispersion and leads to the reduction of the temperature dependence of Δn_2. In the polar phase of KDP crystal the following changes of Δn_i are observed: pressure σ_1 leads to the decrease of Δn_2 and to the increase of Δn_3; pressure σ_2 decreases Δn_1 and Δn_3 and pressure σ_3 increases Δn_1 and Δn_2. The analogous baric changes of the birefringence Δn_i of DKDP crystals in polar phase are investigated. When temperature approaches T_c from the polar phase the temperature sensitivity of the baric changes of Δn_i for KDP grows and for DKDP crystals decrease, respectively.

Uniaxial pressure σ_1 and σ_3 shifts PT points of KDP and DKDP crystals to the low temperatures region with different speeds: $dT/d\sigma_1 = -0.003$ (KDP) and -0.007 (DKDP) K/bar; $dT/d\sigma_3 = -0.007$ (KDP) and -0.012 (DKDP) K/bar. Uniaxial pressure σ_2 shifts PT points to the high temperature region: $dT/d\sigma_2 = 0.008$ (KDP) and 0.011 (DKDP) K/bar.

The "resulting" (hydrostatic) pressure: $dT_c/dp = \sum dT_c/d\sigma_i = -0.002$ (KDP) and -0.008 (DKDP) K/bar shifts the PT points to the low temperature region.

On the basis of the experimental data the temperature changes of the combined piezooptic constants π^0_{12}, π^0_{13}, π^0_{31} and π^0_{32} of KDP and DKDP crystals are studied. When temperature increases from the depth of the ferroelectric phase the constants π^0_{im} for KDP crystal increase and achieve maximum at T_c, while for DKDP crystal the opposite behaviour is observed.

Local magnetic structure of the as implanted ferrit-garnet films

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The magnetic field distribution function on the iron nuclei after different doses of As ion implantation has been obtained. The magnetic fields distribution forms evidences about dominant role of thermal peaks in the implanted layer structure information.

Energy spectrum and density of states of electrons with diagonal disorder on two-dimensional lattice in magnetic field

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The expression for Green functions of electrons on two-dimensional lattice sites has been obtained. The energy spectrum and its damping and the density of states have been calculated in the case when the system consists of two chains of N sites.

Swelling and shrinking of polymer chains in the homopolymer blends

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The radius of gyration, R, of polymer chain in homopolymer blends is studied in the framework of a self-consistent one-loop approximation. We show that polymer chains can shrink or swell in comparison to the Gaussian chain. The swelling of polymer chains in a region far away from the critical point is caused by the steric repulsive forces that were included in the model as constraint of incompressibility. The chains shrink progressively, as we approach the critical region passing through the Gaussian limit, $R_0 = \sqrt{\frac{N}{6}}l$ (N - polymerization index, l - length of monomer), far away from the critical point. The correction responsible for swelling and shrinking is small when concentrations of components $\bar{\phi}$ are comparable ($N = 1000$, $\bar{\phi} = 0.5$, $\frac{R_0^2 - R^2}{R_0^2} = \pm 0.02\%$). This effect, although small, leads to local demixing (sharp shrinking of chains in both component accompanied by strong change of global inter-monomer distance) which should be experimentally observable. When local demixing occurs there is a sudden increase in the scattering intensity (of the order of 30% for $N = 1000$, and $\bar{\phi}_A = 0.2$). The increase of the polymerization index of one component leads to increase of swelling-shrinking effect for this component. In addition, the critical concentration in such system changes towards the smaller value of shorter chains component concentration in comparison to the value obtained in the Flory-Huggins theory. The self-consistent determination of the radius of gyration and the upper wave-vector cutoff makes our model free from any divergences. In the limit of $N \to \infty$ this theory reduces to the RPA of de Gennes.

Gas-liquid phase transition. Van der Waals model

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For the Van der Waals model the kinetic theory of critical phenomena is developed. This approach differs radically from the traditional phenomenological one which is based on the scale-invariance hypothesis and on the renormalization group method. By the analysis of the kinetic equation the account of dynamic and fluctuational characteristics is carried out and on this basis the explanation of some experimental date is given. The dynamical processes is described in the self-consistent approach for the first and the second moments. For the description of fluctuational processes the corresponding Langevin equations are used. The intensity of Langevin sources by the structure of the dissipative terms in the kinetic equation is defined.

The analysis of experimental date on temperature dependence of the thermal capacity and for spectra of molecular scattering of light confirms the theoretical result of the kinetic theory.

Wall-induced lamellar order in microemulsions

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A structure of microemulsion near a planar wall is studied
(1) within a lattice model in which the orientations of amphiphiles are taken into account [1]
(2) within a Landau-Ginzburg model based on a new order - parameter for lamellar ordering.

In the bulk the second- and the first - order transitions between microemulsion and the lamellar phase occur in both models and the wetting of the solid wall by the lamellar phase at coexistence with microemulsion can be studied.

We find:
(a) near the wall the concentration distribution is different from the corresponding correlation function in the bulk.
(b) the closer to the coexistence with the lamellar phase, the more structured the near-surface fluid, i.e. the larger the number of lamella near the surface.
(c) continuous wetting transition by the lamellar phase at coexistence with microemulsion occurs.

Our results are in conformity with recent experimental findings [2,3].

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On the subthreshold defect formation in semiconductor crystals

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The radiation defect formation in solids emerges from the atom displacement and the vacancy-interstitial pair production, which mostly moves over the volume and forms stable secondary defects with impurities and other imperfections. Several mechanisms of radiation defect production have been proposed. The simplest one is the elastic collision, when the energy of atom E_a, transferred from the irradiation is greater than E_d (threshold for adiabatic displacement of the lattice atom).

Under certain condition, a structural defect production and even subthreshold processes will occur. Among several theories in this field the impurity-ionization mechanism (IIM) proposed by Karpov and Klinger should be of vital importance for defect production in non-metallic crystals, particularly in semiconductors and ion crystals. The IIM may be efficient when the energy E_c of the Coulomb interaction between the host atom and impurity atom ions be greater than E_d. The second term which is necessary for IIM is that the time of positive charge localization at the ionized atom is greater than the atom displacement time.

Thus, the realization of the IIM requires adherence of two conditions:

1. The concentration of impurities taking part in defect production is high enough (for example in Ge and Si the donor concentration of P atoms will be more than $5 \cdot 10^{17}$ per cm^{-3}) providing the energy transform via Coulomb interaction.

2. The localization time of the charge at a free ion is larger than atom displacement time.

So, the point is to determine the displacement of different kind of atoms distributed over a single set of sights in the vicinity of ionized atoms.

These conditions are analyzed in detail.

Author's Index

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93-3230	Comparative study of the disorder crystal with phase transitions, the dielectric glasses and the ferroelectric ceramics	Y.Vysochanskii
93-3657 -ext	II-VI semiconductor quantum wells and superlattices	S.Ryabchenko
94-0324	Non-linear optics, lasing, dynamics and localization of excitons in II-VI epilayers and superlattices	M.Brodyn, S.G.Shevel
94-0870	Non-linear phenomena in microphysics of collisionless plasmas, space and laboratory applications	A.Sitenko
94-0935	Magnetoelectric and related physical properties of insulating multiferroic crystals in magnetic fields up to 30 Tesla	N.F.Kharchenko
94-1720	Tunneling of magnetization and electron tunneling that depends upon magnetization in mesoscopic objects	M.Tkach
94-2940	Plasma crystal studies: plasma crystal laser	A.Zagorodny
94-2959	Statistical physics of complex fluids and plasmas	A.Sitenko, A.Zagorodny, Yu.Klimontovich
94-3754	Non-linear modes in quasi-one-dimensional polymers and high-temperature superconductors	I.Baryakhtar
95-0133	Investigation of the complex formation and ionic transport processes in water, aqueous solutions and H-bonded systems for the development of environmental protection solutions connected with water pollution	M.Rasmussen, M.Holovko, I.Stasyuk, M.Tokarchuk, K.Heinzinger, I.Protsykevich, O.Ivankiv, A.Zagorodny
96-0617	Physics and applications of colloidal and dusty plasmas	O.I.Gerasimov, A.Zagorodny

INTAS – the International Association for the promotion of co–operation with scientists from the New Independent States of the former Soviet Union

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INTAS, the International Association for the promotion of co-operation with scientists from the New Independent States of the former Soviet Union (NIS) was established in June 1993 as a European initiative to support research projects and networks of scientific excellence for the mutual benefit of teams from the INTAS members and the NIS. Scientific research projects and networks are selected on the basis of a peer review system from proposals submitted to INTAS in the framework of regularly launched calls, some jointly with other organisations from both NIS and INTAS members. In all cases, INTAS abstains from financing military research and from any political and commercial activities.

INTAS members: Austria, Belgium, Denmark, Finland, France, Germany, Greece, Iceland, Ireland, Israel, Italy, Luxembourg, The Netherlands, Norway, Portugal, Spain, Sweden, Switzerland, the United Kingdom and the European Community.

The National Academy of Sciences of Ukraine

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The National academy of sciences of Ukraine is the highest scientific institution of the country and a one of leading centers of science in the world. The Ukrainian academy of sciences was founded in 1918.

The Academy is a community consisting of nearly 38 thousands of scientists working in more than 130 scientific institutions. It unites more than 13 thousands researchers, among them 2406 doctors and 8207 candidates of sciences.

70% fundamental researches in Ukraine are performed by the Academy's institutions.

The Academy is organised in 13 Divisions devoted to:
- mathematics;
- informatics;
- mechanics;
- physics and astronomy;
- Earth sciences;
- new materials;
- energetics;
- chemistry;
- molecular biology, biochemistry, experimental and clinical physiology;
- general biology;
- economics;
- history, philosophy and law;
- literature, language and art.

The Division of physics and astronomy is one of the largest divisions and posesses the largest intellectual potential. The Division encircles 19 scientific institutions in Kyiv, Kharkiv, Lviv, Donetsk, Uzhgorod and Sumy. 522 doctors and 1434 candidates of sciences work in them.

The Academy coordinates scientific studies via regional scientific centers: Innovative (Kyiv), Western (Lviv), Southern (Odesa), South-Eastern (Kharkiv), Dniprean (Dnipropetrovsk), Crimean (Simferopol) and Donetsk centers.

Ministry of Ukraine for Science and Technology

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Ministry of Ukraine for Science and Technology is a central body of executive power that is providing implementation of state policy in the sphere of scientific and technological activities of the bodies which are administering in scientific and technological spheres; is responsible for development of scientific and technological potential of Ukraine; inspecting an effectiveness of making use of financial and material means assigned by the state for development of science and technology.

Objectives of the ministry

- Establishing principles of scientific and technical development;
- Securing development of scientific and technical potential of Ukraine, taking measures to improve the network of scientific research establishments and organizations:
- Organizing and co-ordinating innovative activities;
- Co-ordinating the development of the national scientific and technical information system;
- Making arrangements for protecting rights to industrial property;
- Managing the activities of the system of scientific and technical expert examination;
- Exercising state supervision and control in the sphere of scientific and technical activities;
- Ensuring integration of the science of our country into world's scientific expanse while preserving and protecting the national priorities.

THE FUNDAMENTAL RESEARCHES STATE FUND

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The Fund celebrated in March, 1998 its 6th anniversary. The most important aim of the Fund – to be the active constituent of the whole innovation cycle (fundamental scientific project – scientific technological project – accomplished innovation) which is carrying out under the guidance of the Ministry of Ukraine for science and technology.

During the time of existence of the Fund 5 competitions of the scientific projects have been carried out. The projects were refereed by about 2000 experts from more than 300 institutions. The grants have been awarded to nearly 10000 winners from all the regions throughout Ukraine.

The list of the works selected in the 4th competition of the Fund includes 728 grant projects involving participants from 231 institutions in Ukraine. It was planned, for 1997, that the means of the Fund reach 9007 thousands hrn., which would constitute 1.3% of the whole amount aimed for the science. The distribution of the costs over the scientific directions of the Fund is as follows: mathematics, mechanics, informatics – 11%, physics and astronomy – 23%, chemistry – 13%, scientific Funds of contemporary technologies – 16%, biology – 13%, earth sciences, cosmology, and environment problems – 11%, fundamental aspects of humanities – 4%, fundamental social–economic problems – 6%, forecasting the development of the science and education – 3%. There is the following departmental distribution of the grants: National Academy of Sciences – 64.2%, Ministry of Education – 21.6%, Ministry of Health Protection – 1.4%, Ukrainian Academy of Agricultural Sciences – 1.3%, other organizations – 11.5%.

To obtain more detailed informations on scientific activities, their participants, and addresses of basic institutions please contact the Ukrainian Ministry of science. We would be glad to meet you in the Fund.

RESEARCH ASSISTANCE FOUNDATION

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Research Assistance Foundation was established in 1996 on the initiative of the Western Scientific Center bureau of the National Academy of the Sciences of Ukraine, Lviv regional administration, under the approval of the President of Ukraine, the Head of the Parliament of Ukraine.

The President of Research Assistance Foundation is Academician, Prof. Ihor Yukhnovskii, a well-known scientist and politician.

The Foundation main goal *is to preserve the existing scientific schools, to support the fundamental researches of the main scientific fields, to enlist youth intensively to scientific researches.*

Objectives of the Foundation

- *To draw institutions and organizations of different forms of property, people for supporting scientific researches of the vital importance.*
- *To assist the forming of new approaches based on the co-responsibility of state, financial, business structures and citizens for the development and outcomes of fundamental scientific researches.*
- *To accumulate the financial, material and other resources in order to direct them at the research and realization of the actual and principal scientific and scientific-and-technical projects and programs.*
- *To carry out the charitable and sponsoring activities on the legal, open and voluntary basis.*

The Advisory group of consultants of the Foundation *defines the list of prospective scientific spheres, gives the final estimation as to expediency of projects implementation. It consists of distinguished scholars and experts in different scientific spheres.*

The funds of the Foundation *are formed of entrance fees of its members voluntary pecuniary payments and assignments from the institutions, enterprises, state and public organizations, as well as citizen and other receipts*

CONDENSED MATTER PHYSICS

The journal is founded in 1993 by the Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine

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Condensed Matter Physics contains original and review articles in the field of statistical mechanics and thermodynamics of equilibrium and nonequilibrium processes, relativistic mechanics of interacting particle systems. Papers are published in English. They are abstracted and indexed in the journals ”Physics Abstracts” and ”Chemical Abstracts”.

You will find a more detailed description on
`http://www.icmp.lviv.ua/icmp/journal/`

- single crystals and films of yttrium aluminum garnet for solid state scintillators;
- single crystals of tungstates and molibdates for detectors of radiation;
- amorphous and vitreous chalcogenide semiconductors;
- heterostructures of A^3B^5 (GaAs-AlGaAs, InP-InGaAsP) and A^2B^6 (CdHgTe) for semiconductor lasers and detectors of visible and IR radiation;
- thermoplastic materials for security, protection and information identification devices;
- lithium niobate and tantalate single crystals for surface acoustic waves filters;
- epitaxial films of garnets and hexaferrites for microwave devices;
- single crystal substrates of rare-earth gallium garnets and epitaxial films of ferrogarnets with bubble domains for memory devices;
- epitaxial films of Bi-substituted ferrogarnets for devices of magneto- and optoelectronics (modulators, deflectors, circulators etc.);
- rare-earth aluminate and gallate single crystal and $ABXO_4$ tetragonal crystal substrates for HTSC films;
- liquid and film adhesives as well as sealants for surface assembly of integrated circuits, electronic devices sealing etc.;
- UV and IR curing compositions for printed circuit boards;
- heat conductive and current conductive rubbers.