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Alexander Davydov

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Program & Proceedings

Kyiv 2012

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Contents

Part 1

Opening Session

October 8, 14:30-17:45

On the significance of the fluctuations of coherent equilibrium positions displacements in atoms at second-order phase transitions

E. N. Myasnikov, Z. P. Mastropas

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Study of a crystal model with wide forbidden zone as a system of charge carriers and phonons with inter-band electron-phonon interaction is performed. Using mathematical method of temperature (Matsubara) quantum Green's functions, which takes into account both quantum and thermal fluctuations [1], temperature dependence of thermodynamic potential of a crystal with strong electron-phonon interaction around the point of second-order phase transition (PT2) [2] was derived. Variation of electron and phonon subsystems states under the strong electron-phonon interaction allows to establish the connection between lattice deformation at $T \to 0$, which appears as a result of phase transition, and change in distribution function of electrons in elementary cell. This change occurs due to admixing of conduction band states to the valence electrons states. It is shown that under the temperature lowering down to the transition temperature, the potential is logarithmically divergent, as in Onsager's solution to Ising model. This potential growth leads to thermodynamic instability of high-temperature phase with respect to coherent displacements of atoms equilibrium positions; the interaction between electron subsystem and these displacements reduces thermodynamic potential.
Obtained results are used to predict the scenario of real PT2 [3]. As $T = T_c$ point is inaccessible, in real PT2 process the total thermodynamic potential cannot rise infinitely with temperature decreasing. Real processes cannot be quasi-equilibrium, in consequence of significant role of fluctuations. Therefore such PT2 can be realized as a first-order fluctuation phase transition at $T_1 > T_c$ with step-wise appearance of finite by the order of magnitude lattice deformation which is stabilized by the electron-phonon interaction.

[1] A.A. Abrikosov, L.P. Gor'kov, I.E. Dzyaloshinskii. Methods of quantum field theory in statistical physics, Nauka, Moscow (1962).
[2] A.E. Myasnikova, E.N. Myasnikov, Z.P. Mastropas, Theoretical and Mathematical Physics, **157** (2), 1595 (2008).
[3] E.N. Myasnikov, Z.P. Mastropas, Physics of the Solid State, **52** (3), 599 (2010).

Double, Double, ... Bubble

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The famous picture of the double helix of DNA is only a static view. The lifetime of a base pair, i.e. the time during which it stays closed, is only of the order of a few milliseconds. At high temperature some parts of the double helix open locally and form the so called "denaturation bubbles", which play a role in biological function.

Thermal denaturation of DNA is a nice subject for theoretical studies, but, what can we say experimentally about them? How can we validate the theories?

We have combined different approaches to study the spatial structure of DNA fluctuations, neutron scattering and the analysis of magnetic birefringence data. However raw data are only useful if they can be analyzed in the framework of a theoretical description. The talk will present the experimental measurements and discuss their analysis.

References:

[1] Andrew Wildes, Nikos Theodorakopoulos, Jessica Valle-Orero, Santiago Cuesta-Lopez, Jean-Luc Garden, and Michel Peyrard, *The thermal denaturation of DNA studied with neutron scattering* PRL **106** 048101-1-4 (2011) and *Structural correlations and melting of B-DNA fibers.* Phys. Rev. E **83** 061923-1-11 (2011)

[2] N. Theodorakopoulos and M. Peyrard *Base Pair Openings and Temperature Dependence of DNA Flexibility* PRL **108** 078104-1-4 (2012)

O-03

Polaron motion in molecular chains and DNA conducting properties

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General properties of electron motion in molecular chains are considered. The charge motion is described in terms of quantum mechanics, whereas vibrational degrees-of-freedom are treated both classically and quantum mechanically. A typical charge transfer/transport pattern can physically be viewed as a polaron and/or soliton. A closed analytical expression for charge carrier velocity dependence on electric field has been derived and analyzed in detail. Special attention is given to: dynamical behavior of electrons in rigid chains, band structure of regular polynucleotide chains, dynamics of polaron states formation in Holstein chain, polaron motion in an electric field, the role of dispersion, Bloch oscillations and breather states, the bipolaron mechanism of a superconducting state in DNA based on Holstein-Habbard model.

[1] V.D. Lakhno, V.B. Sultanov, Chem. Phys. Lett. **503**, 292 (2011).
[2] V.D. Lakhno, A.N. Korshunova, EPJB **79**, 147 (2011).
[3] V.D. Lakhno, Int. Journ. Quant. Chem. **110**, 127 (2010).
[4] V.D. Lakhno, JETP **137**, 926 (2010).
[5] N.I. Kashirina, V.D. Lakhno, Physics-Uspekhi **53**, 431 (2010).

The dynamical chaos phenomenon in a high-energy charged particles passage through a bent crystal

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When a fast charged particle is moving in a crystal near one of the crystal axes it successively collisions with different crystal atomic strings that are parallel to the axis. In such motion the phenomenon of dynamical chaos in particle scattering is possible. It means that the periodicity of the crystal atomic strings location may not have a significant effect on the particle motion [1]. A similar phenomenon is possible when the particles penetrate through the bent crystal atomic strings. This fact enables the possibility for realization of the stochastic mechanism of particle beam deflection by a bent crystal, in which particles follow the bend of the crystal axis [2]. This report presents the overview of results of the comparative analysis of the stochastic and other mechanisms of particle beam deflection by means of a bent crystal [3,4]. The considerable efficiency of the stochastic mechanism to deflect both positively and negatively charged particles is shown. We also discuss recent CERN experiments [5] for the detection of the stochastic mechanism of charged particles deflection.

[1] A.I. Akhiezer, V. I. Truten', N. F. Shul'ga, Physics Reports **203**, 289 (1991).
[2] A.A. Greenenko, N.F. Shul'ga, JETP Lett. **54**, 524 (1991).
[3] N.F. Shul'ga, I.V. Kirillin, V.I. Truten', Phys. Lett. B **702**, 100 (2011).
[4] N.F. Shul'ga, I.V. Kirillin, V.I. Truten', Nuovo Cimento C **34**, 425 (2011).
[5] W. Scandale *et al.*, Phys. Lett. B **680**, 301 (2009).

Part 2

Solid State Theory

09 October, 9:30 - 13:00

Nambu-Goldstone modes of the two-dimensional Bose-Einstein condensed magnetoexcitons with wave vector $\vec{k} = 0$

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The collective elementary excitations of two-dimensional magnetoexcitons in a Bose-Einstein condensate (BEC) with wave vector $\vec{k} = 0$ were investigated in the framework of the Bogoliubov theory of quasiaverages. The Hamiltonian of the electrons and holes lying in the lowest Landau levels (LLLs) contains supplementary interactions due to virtual quantum transitions of the particles to the excited Landau levels (ELLs) and back. As a result, the interaction between the magnetoexcitons with $\vec{k} = 0$ does not vanish and their BEC becomes stable. The equations of motion for the exciton operators $d(P)$ and $d^{\dagger}(P)$ are interconnected with equations of motion for the density operators $\rho(P)$ and $D(P)$. Instead of a set of two equations of motion, as in the case of usual Bose gas, corresponding to normal and abnormal Green's functions, we have a set of four equations of motion. This means we have to deal simultaneously with four branches of the energy spectrum, the two supplementary branches being the optical plasmon branch represented by the operator $\rho(P)$ and the acoustical plasmon branch represented by the operator $D(P)$. The energy spectrum of the collective elementary excitations consists from two quasi-Nambu-Goldstone(NG) modes describing the exciton-type branches (energy and quasi-energy branches), each of them with an energy gap and a roton-type region, from a true NG mode describing the gapless optical plasmon branch and from the acoustical plasmon branch of the NG type wnich reveals the absolute instability in the range of small and intermediary wave vectors.
E.V.D. thanks the Foundation for Young Scientists of the Academy of Sciences of Moldova for financial support (11.819.05.13F).

Breathers in C_{60} Nanocrystals

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We study the dynamics and thermal conductivity of nanoclusters composed of C_{60} fullerene molecules. We reveal that such composite nanostructures can support long-lived strongly localized nonlinear modes, which resemble discrete breathers in simple nonlinear lattices. In these localized modes, the vibrational energy is localized predominantly at one of the C_{60} molecules, and it decays rapidly away from the localization region. Our numerical simulations demonstrate that at room temperatures the lifetime of such nonlinear localized modes may exceed tens of picoseconds. Consequently, we observe that C_{60} nanoclusters demonstrate anomalously slow thermal relaxation in comparison with the nanoclusters composed of carbon nanotubes, and the temperature gradient decays in accord with a power law, thus violating the Cattaneo-Vernotte law of thermal conductivity.

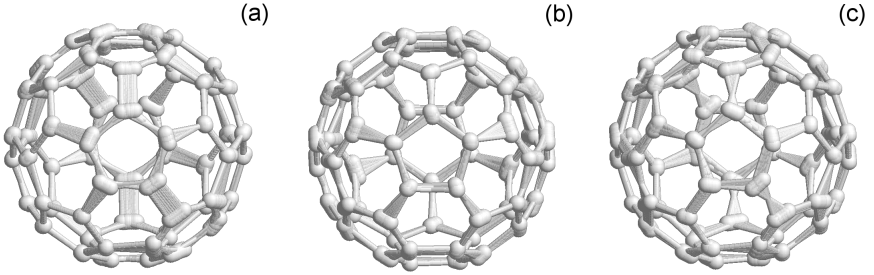

Рис. 2.1: Selected eigenmodes of an isolated C_{60} molecule which lead to the generation of spatially localized nonlinear modes (breathers) of the fullerene crystal. (a) mode $T_{3g}(1)$ (frequency $\omega = 442.3$ cm^{-1}); (b) mode $T_{1g}(2)$ (frequency $\omega = 675.7$ cm^{-1}); (c) mode $T_{1g}(3)$ (frequency $\omega = 1454.9$ cm^{-1}).

[1] A.V. Savin, Y.S. Kivshar, Appl. Phys. Lett. **98**, 193106 (2011).
[2] A.V. Savin, Y.S. Kivshar, Phys. Rev. B **85**, 125427 (2012).

Pecularities of exciton condensed phase manifestation in quantum wells

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The observation of periodical spatial structures in emission excitonic spectra from semiconductor double quantum wells [1,2] aroused an interest of many investigators. Our model[3] for the explanation of the phenomenon is based on two suggestions: a) there is an exciton condensed phase, caused by exciton-exciton interaction, b)the system is non-equilibrium one due to the finite value of the exciton lifetime. The explanation does not need an involvement of the exciton Bose-Einstein condensation. In the report the following results are presented: 1) the influence of a disorder on exciton emission spectra in a condition of the condensation,2)the hydrodynamics equations for excitons in condensed phase, 3) an existence the solitonlike states (excitonic autosolitons) outside the spinodal region.

[1] A.V. Larionov, V.B. Timofeev, J.Hvam, and K. Soerensen, JETP Lett. **71**, 117 (2000).
[2] L.V. Butov, A.C. Gossard, and D.S. Chemla, Nature **418**, 751 (2002).
[3] V.I. Sugakov, Solid State Commun.,**134**,63 (2005);A.A. Chernyuk and V.I. Sugakov, Phys. Rev. B **74**, 085303, (2006);V.I. Sugakov, Phys. Rev. B **76**, 115303 (2007).

Cooperative phenomena in proton conductors (quantum lattice gas approach)

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The description of crystalline ionic, in particular proton, conductors is usually based on the lattice gas models where quantum hopping of particles and their interactions are taken into account. In the case of protons, when they move within the subsystem of hydrogen bonds, the Grotthuss mechanism (the proton tunneling on the bond and hopping between the nearest bonds) is taken into account. We investigate the properties of this model based on the mixed Pauli statistics which makes it similar to the well-known hardcore boson model. We focus on the changes induced by the short-range particle interaction and the inner modulation field in proton spectra and equilibrium states picture.

First, we use the analytical approach based on the random phase approximation to obtain the single-particle spectral densities for various phases of the system. We analyze specific features of spectral densities (an opening or closing of a gap, an appearance of a negative branch) that correspond to the so-called Mott-insulator (MI) state, the superfluid (SF) like state with the Bose-Einstein condensate and the charge density wave (CDW) like state at both zero and finite temperatures. The phase diagrams (μ, T) and (μ, t) for different values of interaction strength and modulation field are built and discussed.

Second, we compare the results of this analysis with the data of numerical calculations which we perform using exact diagonalization technique for finite one-dimensional system of N=10 sites in periodic boundary conditions. We include the short-range interactions between particles as well as the inner modulation field into these numerical calculations and find out their influence on the specific structure of the single particle spectrum which corresponds to a certain state of the system. The corresponding diagrams of state are built and analyzed.

The appearance of SF-like state can be attributed to the superionic phase transition observed in superprotonic conductors such as the $Me_mH_n(XO_4)_l$ (Me = Cs, Rb, NH_4; X = S, Se) family of crystals, while the CDW like state is an analogue of ferroelastic phases in these compounds. From the other hand, the obtained phase diagrams also describe the behaviour of ultra-cold bosonic atoms in modulated optical lattices.

On the utilization of the permutation symmetry instead of translational in the band theory construction of the finite periodic crystals and other structures

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При построении зонной теории для кристаллов конечных размеров и других конечнопериодических структур (кластеров, фуллеренов, фракталов и пр.) в одноэлектронном приближении предлагается использовать группу перестановок вместо группы трансляций. Вводится понятие минимальной ячейки, определяемой как наименьшая часть пространства, задание самосогласованного потенциала в которой достаточно, чтобы посредством операций симметрии полной кристаллической группы получить потенциальное поле всего кристалла. Полная кристаллическая группа состоит из точечной подгруппы и подгруппы циклических перестановок вдоль основных векторов решётки. В этом случае можно доказать и аналог теоремы Блоха.

Analog of the Davydov splitting in the carbon graphene-like structures

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В серії робіт, опублікованих в кінці 80-х років групою співробітників Інституту фізики напівпровідників ім. В.Є.Лашкарьова НАН України (В.І.Гавриленко, В.Г.Литовченко, М.І.Клюй та ін.), було досліджено оптичні властивості двомоношарових графеноподібних структур, вуглецю [1]. Теоретичні спектри були отримані в рамках наближення сильного (вздовж кожного шару) зв'язку, експериментальні дослідження проводились методом оптичної модуляційної спектроскопії та ІЧ спектрів поглинання. Основну увагу було зосереджено на незвичайних явищах, що виникли завдяки відхиленню від ідеальної кристалічної гратки, а саме, спостереженню змін під дією деформацій чи легування. Принциповим виявилось поява щілини в безщілинній κ-точці забороненої зони (**??**), а також зсув в інших (Г, Н) характеристичних точках 33, причому саме в бік збільшення енергій. Рис. 1. Цей ефект був інтерпретований як виникнення додаткової гібридизації валентних зв'язків з залученням до $sp2$ гібридів певної долі $sp^2_{xy}p_z$, тобто $sp3$ гібридів, які мають, в ідеальному випадку, тетрагональну алмазоподібну конфігурацію з підвищеною величиною енергії зв'язку (аж до "алмазних величин»). Ці факти, згодом, стали базовими для формування окремого напрямку інженерії нового класу напівпровідників - зі зміною 33, причому без зміни хімічного складу речовин [2].

Поза увагою, однак, тоді виявились ще декілька важливих результатів цих робіт, а саме 1) лінійний характер закону дисперсії в точці «злипання» зон , тобто для точки к, 2) розщеплення зонної структури на дві. Перший факт став згодом загальновідомим для ідеальної одно-моношарової графенової структури в циклі знакових робіт по графеновій тематиці [3], і знайшов пояснення на базі ставших вже класичними уявлень.

В даному повідомленні ми звертаємо увагу на факт розщеплення зон, що має місце без будь-яких деформацій чи відхилень від ідеальної структури.

Використовуючи значення параметрів для добре експериментально дослідженого тонкоплівкового графіту (відстань між шарами $h = 2,6\AA$) , ми отримали з розрахунків значні величини розщеплення зон для всіх критичних точок зони Бриллюена цієї дво-моношарової структури. Ці дані ілюструються на Рис.1 та в Табл.1.

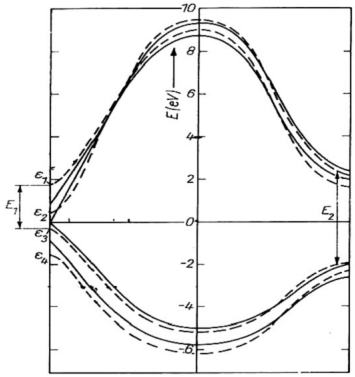

Рисунок 2.2: Зонна структура двохшарового графеноподібного вуглецю (пунктир – при деформації) [1]

Type of point	ΔE_C	ΔE_V	ΔE_g	ΔE_{CD}	ΔE_{VD}	ΔE_{gD}
	eV					
k	1	0,8	1,8	1,7	1,3	3,30
Γ	-0,8	-0,9	0,3	0,6		-0,6
M	-0,5	-0,5	0,2			-0,5

Табл.1. ΔE_C *splitting for different energy bend critical points.*

Як відомо, Давидовське розщеплення виникає завдяки резонансної взаємодії між двома однаковими сусідними молекулами «молекулярного кластера» , одна з яких знаходиться в основному Ψ_0 , а інше – в збудженому Ψ стані. Виникає поправка до енергії системи такого диполя вже в 1-му наближенні теорії збудження. Причому

$$\psi_n \left| r \right| \Psi_0 > \$$$

$$\Delta E_1 \left(R \right) = -\Delta E_2 \left(R \right) = \frac{e^2}{R_3} \quad (1,2)$$

де $\Phi(1,2) = \phi(\Delta\theta_{1,2})$ – геометричний фактор, що задається різною орієнтацією

дипольних переходів обох молекул θ_1,θ_2 (споріднених кластерів кристалоструктури). При $\theta_1 = \theta_2$ маємо $\Phi(1,2) = 0$.
Квадрат матричного елементу $I \dots I$ дипольного переходу був оцінений О.С.Давидовим через силу осцилятора відповідного переходу fno та циклічну частоту переходу $\omega = (E_n - E_O)/h$ у вигляді (m – ефективна маса електрона):

$$|\varphi_n |r| \varphi_0|^2 = \frac{\hbar \cdot f_{no}}{2\mu \cdot \omega}$$

,

$$\Delta E = \frac{e^2\hbar}{m\omega R^3}\phi(1,2) \sim \frac{1}{R^3}.$$

На відміну від випадку сил Ван-дер-Ваальса, де $\Delta E \sim 1/R^6$ і швидко спадає з відстанню між молекулами, маємо досить сильну взаємодію між молекулами бі- структури двошарового графіту.
Особливості резонансної взаємодії в цій структурі, згідно Давидову, полягає в тому, що в кожному з обох станів енергія збудження в любий момент часу з однаковою ймовірністю розподілена між обома узагальненими молекулами, отже є спільна для системи, розщепленої на два стани Ψ_1 та Ψ_1 , а хвильова функція системи є суперпозиція, що задається періодичною в часі функцією

$$\psi_E = \frac{1}{\sqrt{2}}(\psi_1 + \psi_2) \sim \phi F(\exp(-it/\tau))$$

У випадку дво(декелька)-моноатомношарових вуглецевих структур вона уявляє з себе шаруватий кристал з відносно невеликою міжшаровою відстанню R˜0,40 nm, отже, тут передбачається досить велика енергія розщеплення, як це і проілюстровано в таблиці.

1. V. Gavrilenko, N. Klyui, V. Litovchenko, et.al. Characteristic Features of the Electronic Structures of Carbon Films, Phys.Stat.Solidi B145, 209-217 (1988)

2. Lytovchenko V.G., Strikha M.V., Klyui M.I. Modified Graphene-like Films as a New Class of Semiconductors with a Variable Energy Gap Ukr. J. Phys. 2011, Vol. 56, N 2, p.175-178

3. A. Geim, Science 324, 1530 (2009)

Spin-dependent transport in graphene and carbon nanotubes doped with chromium

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A method is developed self-consistent calculation of the energy spectrum of the free energy and electric disordered crystal. Taken into account the processes of electron scattering on the ion core potentials of different sort and lattice vibrations. Electronic states of the system described in the self-consistent tight binding model. Obtained cluster expansion for the density of states, free energy and electrical conductivity of disordered system. It is shown that the contributions of scattering processes of elementary excitations in clusters decreases with increasing number of sites in the cluster for some small parameter. Investigated the energy spectrum of electrons and phonons of graphene and carbon nanotubes doped with chromium. Done geometric optimization of the crystal structure of graphene and carbon nanotube chirality (3.0) with a chromium impurity by minimizing the free energy. The influence of chromium impurity on splitting energy bands of electrons and phonons is caused by non-equivalent position of carbon atoms in the primitive cell of graphene and carbon nanotubes. Found out the nature of the spin-dependent electron transport of graphene and carbon nanotubes with chromium atoms, adsorbed on the surface. It is shown that the value of the spin-dependent transport is associated with a relative shift in the external magnetic field energy levels of electrons (the Coulomb gap, resulting in the Fermi level) for different spin projections.

Superfluidity of spatially-indirect magnetoexitons in topological insulators

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We present a theory of magnetoexciton supefluidity in topological insulator (TI) heterostructures. Two systems - a TI film on a dielectric substrate and a sandwich TI - dielectric film - TI are considered. The systems are subjected by a quantizing magnetic field applied perpendicular to the TI - dielectric (TI-D) interfaces. It is implied that the Fermi level is tuned close to the Dirac point of the TI surface state spectrum. Here indirect excitons are understood as bound pairs of a filled and empty quantum states in zero Landau level at adjacent TI-D interfaces.
The approach is similar to one developed for graphene heterostructures [1]. The difference between graphene and TI systems is the presence of only one Dirac cone in the spectrum of TI-D interface states, in difference with 4 such cones for graphene. This distinction allows to avoid of use electrical gates for TI heterostructures (in graphene structures magnetoexciton superfluidity can be realized only in system subjected by a rather strong electrostatic field parallel to the magnetic field [1]).
The dependence of the temperature of superfluid transition T_c on magnetic field B is shown in Fig. 1. TI with dielectric constant $\varepsilon_{TI} = 100$ is considered. Dielectric constant ε_D for the substrate (dielectric film) varies as given in figure caption.

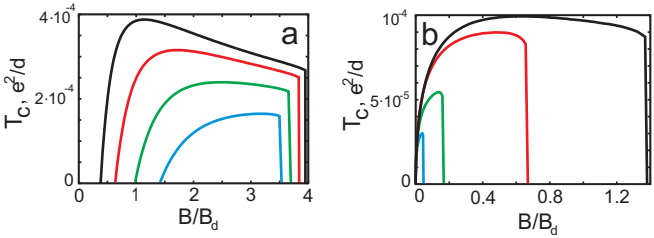

Рисунок 2.3: Critical temperature. $B_d = \phi/\pi d^2$, $\phi = hc/2e$, d is the distance between adjacent TI-D interfaces. a. TI film on a substrate with $\varepsilon_D = 5, 10, 20, 40$ (upside down) , b, TI-D-TI sandwich with $\varepsilon_D = 100, 50, 20, 10$ (upside down).

[1] A.A. Pikalov, D.V. Fil, Nanoscale Research Lett.: **7**, 145 (2012).

Part 3

Physics of Biological Macromolecules

9 October, 14:30 - 18:20

O-13

Conformational solitons work in DNA

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The DNA macromolecule is a polymorphic structure with a variety of the double helix conformations. Natural polymorphism of the double helix and the cooperativity of conformational transformations make very probable the formation of nonlinear excitations on conformational degrees of freedom. As known, the conformational transformations in double helix may induce the deformation of the macromolecule as a whole, and in opposite - the deformations of the DNA backbone may reflect in the conformational state of the double helix. The interrelation between internal and external degrees of freedom of the macromolecule and the polymorphic properties of the monomer unit of DNA chain are the main nonlinearities of the system.
The analysis of the localized excitations occurrence in DNA double helix show, that the dynamical conformational solitons may exist in the stressed macromolecule. The conformational soliton is dynamically stable and can propagate along a macromolecule with a supersonic speed, as a specific signal for the activation processes of genetic information transfer [1].
The static localized excitations can be formed in conformational bistable fragments of the double helix under definite external conditions. The static excitations may take the form of a bell or a step for the conformation component, and may induce the bending and (or) torsion deformation of DNA backbone. The static conformational solitons may serve as DNA specific sites for proteins recognition [2,3].
The conformation solitons work also in the cooperative processes under DNA threshold deformations (double helix unzipping and overstretching), which occur under action of external forces. The proposed mechanism includes the cooperative transition of the double helix in the metastable state at some critical value of external force, and the propagation of the related deformation along the macromolecule as a solitary wave [4]. For DNA unzipping process the transition metastable state was found in SMD simulations [5], confirming the soliton model of threshold deformations.

[1] S.N. Volkov, J. Theor. Biol. **143**, 485 (1990).
[2] S.N. Volkov, J. Biol. Phys. **31**, 323 (2005).
[3] P.P. Kanevska, S.N. Volkov, Ukr. J. Phys. **51**, 1001 (2006).
[4] S.N. Volkov, A.V. Solov'yov, Eur. Phys. J. D **54**, 657 (2009).
[5] S.N. Volkov, E.V. Paramonova, A.N. Yakubovich, A.V. Solov'yov, J. Phys.: Condens. Matter. **24**, 0351043 (2012).

Unveiling the mystery of the DNA overstretching transition

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Torsionalyy unconstrained double-stranded DNA with open ends or nicks undergoes an "overstretching" transition at around 65 pN which leads to DNA elongation of 1.7-fold. Recent experiments from our and other labs have reported that it involves two distinct structural transitions: a hysteretic "strand-peeling" of one strand from the other to an ssDNA strand under tension, and a non-hysteretic "B-to-S" transition to a mysterious double-stranded DNA form often referred as "S-DNA"[1,2]. Here, we show that these two transitions have distinct entropy changes: the entropy change in the strand-peeling transition is positive and the value agrees with that measured in transitional DNA melting experiments; while the entropy change in the "B-to-S" transition is negative and is about one order of magnitude smaller [3]. The salt dependence of the transition shows that the two strands in the "S-DNA" is at close proximity from each other with an inter-strand distance shorter than one Debye-Hückel length [3]. Together with the measured force responses of the ssDNA and the "S-DNA", a force - temperature phase diagram involving three DNA states (B-DNA, ssDNA, and "S-DNA") and a temperature - ionic strength diagram demonstrating the selection between the two transitions are calculated. Finally, repeating similar experiments on end-closed, torsionally unconstrained DNA, we show that the "S-DNA" cannot be an internally melted DNA [4]. Our results prove that a stable S-form DNA exist.

[1] H. Fu,$\cdots$, J. Yan, Nucleic Acids Research: **38**, 5594 (2010). [2] H. Fu,$\cdots$, J. Yan, Nucleic Acids Research: **39**, 3473 (2011).
[3] X. Zhang,$\cdots$, J. Yan, PNAS: **109**, 8103 (2012).
[4] X. Zhang, $\cdots$, J. Yan, to submit (2012).

Radiation damage in biomolecular systems: multiscale approach

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The multiscale approach to the assessment of radiation damage consequent to irradiation by ions was designed in order to qualitatively and quantitatively describe effects that take place when energetic ions interact with living tissues. A road to the understanding physical aspects of ion-beam cancer therapy (IBCT) on the microscopic level revealed that this problem has many temporal spatial, and energy scales, while the main events leading to the cell death happen on a nanometer scale. This approach has become interdisciplinary since it has addressed the key issues of physical, chemical, and biological sciences related to IBCT. Therefore, it is not surprising that this method lies in the core of the COST Action MP1002, Nano-scale insights into IBCT, started in December, 2010, see
http://fias.uni-frankfurt.de/nano-ibct/
http://www.cost.esf.org/domainsactions/mpns/Actions/nano-ibct/ ,
In my talk I would like to introduce the approach and to present the recent results obtained on its basis [1-7]. Finally, I would like to devote some attention to the development of the software package MBN (Meso-Bio-Nano) Explorer, see
http://www.mbnexplorer.com/ ,
which might become a very useful tool in the exploration of radiation damage phenomena on the molecular level.

[1] E. Surdutovich, O. Obolensky, E. Scifoni, I. Pshenichnov, I. Mishustin, A.V. Solov'yov, and W. Greiner. Eur. Phys. J. D 51, 63 (2009).
[2] A. V. Solov'yov, E. Surdutovich, E. Scifoni, I. Mishustin, and W. Greiner. Phys. Rev. E 79, 011909 (2009).
[3] E. Scifoni, E. Surdutovich, and A.V. Solov'yov, Phys. Rev. E 81, 021903 (2010).
[4] E. Surdutovich, A. Yakubovich, and A.V. Solov'yov, Eur. Phys. J. D 60, 101 (2010).
[5] M. Toulemonde, E. Surdutovich, and A.V. Solov'yov, Phys. Rev. E 80, 031913 (2009).
[6] E. Surdutovich, A.V. Solov'yov, Phys. Rev. E 82, 051915 (2010).
[7] E. Surdutovich, D.C. Gallagher, and A.V. Solov'yov, Phys. Rev. E84, 051918 (2011)

Excitation Migration, Quenching and Regulation of Photosynthetic Light Harvesting of Photosystem II

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In order to control the excitation density in oxygen evolving photosystem II (PSII), a physiologically important strategy to regulate photosynthetic light harvesting has evolved by plants resulting in so-called non-photochemical quenching (NPQ) of excitations. This rapid regulation of the excitation density is usually attributed to additional trapping centers generated in the light-harvesting system of PSII under high excitation conditions. Despite recent extensive discussions about the origin of the NPQ-traps, a common agreement has not been achieved so far.

The excitation kinetics in the aggregates of the photosynthetic light-harvesting complexes of PSII (so-called LHCII) under NPQ conditions will be considered. Special emphasis will be paid to the possibility to discriminate between the two limiting cases: migration-limited vs trap-limited. On the basis of this analysis a possible specific mechanism responsible for the quenching process taking place in NPQ will be discussed. For this purpose the exciton dynamics including relaxation to the ground state in a heterodimer will be examined. The heterodimer is chosen to be asymmetric in excitation and reorganization energies, transition dipole moments and excited state lifetimes. The possible role of such a dimer as an excitation quenching center is analyzed.

Recent time-resolved studies of the single LHCII complexes have revealed that despite the continuous illumination the fluorescence intensity from distinct LHCIIs switches rapidly between strong and weak emission levels. To explain these experimental observations a diffusion-controlled model that describes the essential protein dynamics underlying this switching is suggested. The model is based on the assumption that the switching behavior of the LHCIIs reflects a specific intrinsic property determined by the lability and adaptability of the protein scaffold. It is assumed that, depending on the protein structural arrangement, the LHCII trimer can be found in one of two states, corresponding to either a high or a low fluorescence intensity level. Switching between these states is driven by two-dimensional diffusion on the energy surface, with one coordinate reflecting fast molecular vibrations and another determining slow structural changes of the protein. This ability of LHCII to act as an envi-

ronmentally controlled switch that exhibits fast and reversible transitions between almost perfect light-harvesting and quenching states makes it a probable candidate to govern non-photochemical quenching. It seems likely that other allosteric proteins apply a similar switching mechanism.

Dynamics of Davydov Ansätze in light-harvesting complexes of purple bacteria

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A Hierarchy of Davydov trial states are adopted in the Frenkel-Dirac time-dependent variation to study energy transfer dynamics in single-ring and double-ring light-harvesting systems in purple bacteria [1-4]. As a comparison, the Haken-Strobl model is also used. It is found that inclusion of long-range dipolar interactions in the two methods results in significant increases in intra- or inter-ring exciton transfer efficiency. The dependence of exciton transfer efficiency on trapping positions on single rings of LH2 (B850) and LH1 is similar to that in toy models with nearest-neighbor coupling only. However, owing to the symmetry breaking caused by the dimerization of BChls and dipolar couplings, such dependence has been largely suppressed. In the studies of coupled-ring systems, both methods reveal interesting role of dipolar interaction in increasing energy transfer efficiency by introducing multiple intra/inter-ring transfer paths. Importantly, the time scale ($\sim 4ps$) of inter-ring exciton transfer obtained from polaron dynamics is in good agreement with previous studies. In a double-ring LH2 system, non-nearest neighbor interaction can induce symmetry breaking which leads to global and local minima of the average trapping time when there is a non-zero dephasing rate, suggesting that environment helps preserve quantum coherent energy transfer. In contrast, dephasing comes into play only when the perfect circular symmetry in the hypothetic system is broken. This study reveals that dipolar interactions between chromophores may play an important role in the high energy transfer efficiency in the LH2 and other natural photosynthetic systems.

[1] A.S. Davydov, *Solitons in Molecular Systems* (Reidel, Dordrecht, 1985).
[2] J. Ye, K.W. Sun, and Y. Zhao *et al.*, J. Chem. Phys. **137** (2012) (in press).
[2] J. Sun, B. Luo, and Y. Zhao, Phys. Rev. B **82**, 014305(2010).
[3] B. Luo, J. Ye, C.B. Guan, and Y. Zhao, Phys. Chem. Chem. Phys. **12**, 15073(2010).

Transitions of the γ angle in the sugar-phosphate DNA backbone and indirect protein-DNA recognition

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Deformations of sugar-phosphate DNA backbone can contribute to protein-DNA indirect or shape recognition, fine-tuning of DNA-protein molecular interface and facilitate interactions with proteins during complexation. In the present study a set of protein-DNA complexes from NDB data base were analyzed with the aim to investigate the role of variations in the sugar-phosphate backbone for DNA-proteins interactions. The main question is how the transitions of the γ angle in the sugar-phosphate backbone affect the local DNA interface accessible for interactions with proteins. We have shown that transitions from canonical gauche+ (g+) to alternative gauche- (g-) or trans (t) conformations of γ angle lead to changes in the polarity of the DNA accessible surface in both grooves. The sequence-specificity of these changes can facilitate indirect readout in the protein-DNA complexes. The analysis of the protein-nucleic acid interactions we have done evidences that in addition to a higher propensity of nucleotides with A-like sugar pucker to interact in the minor groove as compared with B-like pucker, the A-like nucleotides with t angle γ state interact with proteins more actively than with the g+ angle γ state in both minor and major grooves. The combination of B-like sugar pucker and t state of the γ angle also appeared to be favorable for making protein-nucleic acid contacts in both grooves, especially for Cyt, while the g- angle γ state was less favorable for protein-DNA interactions especially in the minor groove. The possible role of the angle γ transitions in the process of protein-DNA interactions is illustrated using several specific complexes from our database as examples.

Manifestations of ion-phosphate vibrations in the low-frequency Raman spectra of DNA

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The DNA double helix is a polyelectrolyte macromolecule with the negatively charged phosphate groups of the backbone that are neutralized by counterions from the solution. Under high concentration of coutnerions almost all phosphate groups are neutralized, therefore the counteions and phosphate groups form a regular structure along DNA double helix. Such a structure may be considered as ionic lattice (ion-phosphate lattice) [1-3]. The modes of DNA ion-phosphate lattice are prominent in the low-frequency spectra (<200 cm^{-1}) and characterize the state of the double helix backbone and type counterions. The goal of the present work is to determine the counterion vibrations in low-frequency spectra of DNA for the case of different conformational states of the double helix and different counterion types.
Conformational vibrations of DNA with counterions are studied within the framework of phenomenological approach developed [1-3]. The counterions are considered to be localized in two possible positions: near the phosphate groups of the double helix backbone, and between the phosphate groups in DNA minor groove. The double helix in righthanded B-form and lefthanded Z-form are studied. The of calculated spectra for B-DNA with Na^+, K^+, Rb^+, Cs^+, and Mg^{2+} counterions consists of intensive modes of internal conformational vibrations of the double helix (from 10 to 100 cm^{-1}) and the modes of ion-phosphate vibrations (from 100 to 170 cm^{-1}). In case of heavy counterions (Rb^+, Cs^+, and hydrated Mg^{2+}) the modes of ion-phosphate vibrations are rather intensive, while in case of light counterions (Na^+ and K^+) these modes are weak. The comparison of obtained frequencies for conformations of DNA with the experimental data [4] show that the specific modes of Z-DNA are localized near 40 cm^{-1} and characterizes the longitudinal vibrations of nucleosides. The obtained low-frequency Raman spectra provide a way to determine the type of counterions, its position with respect to phosphate groups, and the state of the DNA double helix.

[1] S.M. Perepelytsya, S.N. Volkov, Eur. Phys. J. E. **24**, 261 (2007).
[2] S.M. Perepelytsya, S.N. Volkov, Eur. Phys. J. E. **31**, 201 (2010).
[3] S.M. Perepelytsya, S.N. Volkov, J. Molec. Liq. **164**, 113 (2011).
[4] T. Weidlich, *et all.* J. Biomolec. Struct. Dyn. **7**, 849 (1990).

New approach to the description of thermodynamic properties of water

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Surprising properties of water remain to be in the limelight of many investigations. This is the consequence of nontrivial intermolecular interactions between water molecules. At the same time it had been shown in [1,2] that the specific volume and evaporation heat of water are similar to that for argon. This very surprising fact has natural explanation if the rotational motion of water molecules will be taken into account. Due to rotational motion the bare intermolecular potential undergoes to self-averaging [3]. It is shown that the averaged potential takes the Lenard-Jones form. It is necessary condition for similarity of thermodynamic properties for water and atomic liquids of argon type. The correct values for the temperatures of the critical and triple points are obtained. It is shown that H-bond contributions to the thermodynamic potentials are weak and can be taken into account by the perturbation theory. All thermodynamic properties are reproduces quite correctly.
Weighty arguments about the existence of the dynamic phase transition in water at $T_H \approx 42^0 C$ are given in the work [4,5]. The essential change of the character of the thermal motion takes place at this temperature: the crystal-like character transforms to argon-like one. This phenomenon is manifested in peculiarities of the quasi-elastic incoherent neutron scattering, as well as in the behavior of the isothermal compressibility, the entropy diameter for the vapor-liquid coexistence curve, shear viscosity and other properties.

[1] A.I. Fisenko, N.P. Malomuzh, A.V. Oleynik, Chem.Phys.Lett. **450**, 297 (2008).
[2] L.A. Bulavin, A.I. Fisenko, N.P. Malomuzh, Chem.Phys.Lett. **453**, 183 (2008).
[3] S.V. Lishchuk, N.P. Malomuzh, P.V. Makhlaichuk, Phys.Lett.A **374**, 2084 (2010).
[4] S.V. Lishchuk, N.P. Malomuzh, P.V. Makhlaichuk, Phys.Lett.A **375**, 2656 (2011).
[5] L.A. Bulavin, N.P. Malomuzh, JML (Letter to the Editor) **124**, 136 (2006).

Part 4

Statistical Physics and Kinetics

10 October, 9:30 - 12:50

Unified description of transitional and diffusional processes in statistical systems

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The unified description of diffusion processes that cross over from a ballistic behavior at short times to normal or anomalous diffusion (sub- or superdiffusion) at longer times is constructed on the basis of a non-Markovian generalization of the Fokker-Planck equation. The necessary non-Markovian kinetic coefficients are determined by the observable quantities (mean- and mean square displacements). Solutions of the non-Markovian equation describing diffusive processes in the physical space are obtained. For long times these solutions agree with the predictions of continuous random walk theory; they are however much superior at shorter times when the effect of the ballistic behavior is crucial. An extension of the employed approach for higher spatial dimensions is used to study the implications of hydro- dynamic interactions on the shape of the PDF.

Tensor network description of quantum rings

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Renormalization of tensor networks plays an ever increasing role in the numerical understanding of strongly interacting quantum many-body systems. Such procedures emerged in the tradition of the successful density-matrix renormalization group (DMRG) method introduced by Steven White in the early 90ies of the last century and combine recent insight from quantum information theory with modern numerical techniques. Typically such methods at present are most successful in one an two dimensions, but still require quite substantial computing resources and a major issue is to find the proper algorithm for a given problem.
In our presentation we provide a brief overview about current tensor renormalization methods and apply a new technique for the renormalization of systems with periodic boundary conditions to electronic quantum rings.

O-23

Kinetic equations for the coupled microscopic and macroscopic quantum systems

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Nonequilibrium density matrix method is used to derive a generalized master equation (GME) for the density matrix $\rho(t)$ of the quantum system affected by a high-frequency stochastic field. It is shown that just to the stochastic field the GME is transformed into the Markov's operator equations for the diagonal, $\rho_d(t)$, and off-diagonal, $\rho_{nd}(t)$, parts of density matrix $\rho(t)$. Such a separation allows one to derive a linear balance-like equation for the averaged state populations $P(a;t) = \overline{\langle a|\rho(t)|a\rangle} = \overline{\langle a|\rho_d(t)|a\rangle}$ of the system. Special attention is payed to the system which contain different type of subsystems so that a state of quantum system $a = a_1 a_2 ... a_N$ is expressed via quantum states a_j related to each jth subsystem. Dependently on the type of interaction in the common system, kinetic equation for the $P(a;t) = P(a_1 a_2, ...a_N; t)$ can be transformed into the set of linear kinetic equations for the partial populations $P(a_1 a_2 ... a_j; t) = \sum_{a(\neq a_1 a_2 ... a_j)} P(a_1 a_2, ...a_N; t)$ including the kinetic equation for the separate state populations $P(a_j; t) = \sum_{a(\neq a_j)} P(a_1 a_2, ...a_N; t)$ of the jth subsystem. When interaction between the subsystems can be considered as a perturbation, then above set of linear kinetic equations can be reduced to the set of nonlinear kinetic equations describing a time behavior of subsystem populations $P(a_1; t), P(a_2; t), ...P(a_N; t)$. The order of nonlinearity is dictated by the couplings between the subsystems. In the simplest case of two interacting subsystems, the equations are of the second order. Special situation appears when a common system contains microscopic and macroscopic subsystems. If macroscopic subsystems are supported in a stationary regime then a nonlinearity in the kinetic equations for microscopic subsystems is essentially reduced up to a linear one. As an example, a quantum system that involves two macroscopic electrodes and the molecule embedded between the macroscopic electrodes, is considered in the condition of charge transmission from one electrode to another. The closed set of kinetic equations for populations of molecular electronic states is derived along with respective transfer rates [1-4].

[1] E.G. Petrov, Chem. Phys.: **326**, 151 (2006).
[2] E.G. Petrov, V. May, P. Hänggi, Phys. Rev. B: **73**, 045408 (2006).
[3] E.G. Petrov, V.I. Teslenko, Chem. Phys.: **375**, 243 (2010).
[4] E.G. Petrov, Ukr. J. Phys.: **56**, 721 (2011).

O-24

Shielding of a moving dust grain in a weakly ionized plasma

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Shielding of an absorbing dust grain, that moves with constant velocity in a weakly ionized plasma, is an important problem of dusty plasma theory. Under typical laboratory dusty plasma conditions, the polarization force arising due to plasma anisotropy around the moving grain makes significant contribution to the total ion drag force. A knowledge of the ion drag force as a function of the plasma parameters is necessary for understanding of many dusty plasma experiments, e.g., the anomalous grain heating observed in [1]. It has been shown recently by different authors [2-4] that the ion drag force acting on an absorbing grain in highly collisional plasma can decrease substantially in comparison with the force acting on the grain in collisionless limit and can even change sign, i.e., can be directed along the grain motion. Thus, collisions in plasma (mainly ion-neutral collisions) have a great influence on the ion drag force acting on the dust grain. In the present work, shielding of a moving dust grain in a weakly ionized plasma is studied for a wide range of collisional regimes. The problem is considered on the basis of the Vlasov-BGK equations, which are solved numerically on parallel processors by means of a high-order finite-volume method. The values of the ion drag force, distributions of the electric potential, and basic macroscopic parameters of plasma particles are obtained. In the collisionless limit, our results are found to be in good agreement with those computed using the binary collision formalism [5]. For the collisional-dominated plasma, it is shown that the ion drag force can be negative, i.e., directed along the grain motion. In addition, applicability of analytical models proposed in [3,4] is examined.

[1] A. Meltzer, A. Homann, and A. Piel, Phys. Rev. E 53, 2757 (1996).
[2] L. Patacchini and I.H. Hutchinson, Phys. Rev. Lett. 101, 025001 (2008).
[3] S. A. Khrapak et al., J. Appl. Phys. 101, 033 307 (2007).
[4] A. V. Filippov et al., JETP 108, 497 (2009).
[5] S. A. Khrapak et al., Phys. Plasmas 12, 042308 (2005).

Perturbation theory in the dynamics of liquids

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Within the generalized collective mode (GCM) approach [1] the problem of calculations of equilibrium time correlation functions (TCFs), being interesting from the experimental point of view, can be reduced to the eigenvalue problem for so-called generalized hydrodynamic matrix (GHM). The dimensionality of this matrix depends directly on the number of dynamical variables used for the description or, in other words, on the precision needed from the theory. For instance, in the case of simple fluids the five-variables (nine-variables) GCM scheme allows us to obtain the dynamic structure factor in the form that reproduces explicitly the sum rules up to the fourth (eighth) order including. For multicomponent fluids the dimensionality of the GHM increases drastically, and the problem can be solved only numerically. However for many applications it is important to have the analytical expressions that allows to separate the contributions from different collective excitations.
Several versions of perturbation theories for the GHM eigenvalue problem are developed [2]. In the long-wave-vector limit $k \to 0$ as a small parameter one can use k value. This allows to derive the analytic expressions for all the hydrodynamic TCFs of a multicomponent mixture. In particular, this gives the expressions for dynamic structure factors that are exact in the hydrodynamic limit. Beyond the hydrodynamic region there is another way for the theory development that allows one to take into account cross-correlation effects for bare eigenvalues, calculated for separated subsets of dynamic variables. A few examples of the perturbation theory applications, obtained in the second order, are presented. In particular we perform a comparative study of binary fluids of neutral and charged particles. Specific features in the collective behavior of ionic liquids, caused by the Coulomb interactions, are discussed. It is shown that the cross-correlations between acoustic and optic-like collective modes play an important role in binary mixtures beyond the hydrodynamic region. The obtained results are compared with the others known in the literature.

[1] I.M. Mryglod, I.P. Omelyan, M.V. Tokarchuk, Mol. Phys. **84**, 235 (1995); I.M. Mryg
Condens. Matter Phys. **1**, 753 (1998).
[2] I. Mryglod, R. Folk, S. Dubyk, Yu. Rudavskii, Physica A **277** 389 (2000); I.M. Mryglod, V.M. Kuporov, Ukr. J. Phys. **55** 1172 (2010).

Helons and heat capacity singularity in superfluid helium

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The new type of quasiparticles - "helon"is introduced for description of the experimental observations of the non-elasic neutron scattering in superfluid helium. We proceed from the idea that in the theory of superfluidity Landau [1,2] spectrum of elementary excitations in the normal component should depend on temperature. This statement leads to generalization of the Landau criterion of superfluidity. On this basis, taking into account the experimental data on the dynamical structure factor, we show that in superfluid helium, besides the phonon-roton branch of elementary excitations, there is also the another spectrum with a temperature-dependent gap (see, e.g., [3]). Similar type of excitations, however independent from temperature, has been postulated by Landau in [1] (1941) in parallel with the phonon spectrum and can be qualified as the "Landau rotons"(in contrast with the well known rotons, introduced by Landau later [2] and existing as a part of the single phonon-roton excitation branch). The helons exist in parallel with the phonon-roton excitations, but in contrast to ones, helons disappear at the temperature of superfluid transition T_c. The helons exist only below T_c due to proportionality of the correspondent helon gap $\Delta^{(h)}(T)$ to the condensate density $n_s^{\gamma}(T)$ [4]. This circumstance is the characteristic property of helons, which leads in theory to the singular behavior of heat capacity, well known as the λ - point, at the temperature limit $T \to (T_c - 0)$. The experimental manifestation of helons is in [5].

[1] L.Landau, J.Phys. (USSR) 5, 51 (1941)
[2] L.Landau, J.Phys. (USSR) 11, 205 (1947)
[3] S.A.Trigger and P.P.J.M.Schram, Physica B228, 107 (1996)
[4] V.B.Bobrov, S.A.Trigger, and I.M.Yurin, Phys.Lett. A374, 1938 (2010)
[5] N.M.Blagoveshchenskii et al., Sov.Phys. JETP Lett. 31, 4 (1980)

Fluid interfaces: Fluctuations and confinement effects

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We have developed a field theory approach of statistical physics for the description of neutral, charged and anisotropic fluids in confinements. At the vicinity of simple interfaces, that is surfaces which only effects is to confine the fluid, we have found a general depletion phenomenon of the density profiles and the attraction between two surfaces. These effects are described in a very case where no effect is predicted at the mean field level. The density profiles predicted verify the density contact theorem as well as a new charge contact theorem in the case of ionic fluid.
The developed formalism shows that these effects are due to fluctuations via entropic coupling. We show that these contributions do not depend on the sign of interaction. Therefore they always correspond to a depletion effect. These depletion phenomena can explain simply some unexpected behaviours like the anomalous electric capacitance behaviour as a function of temperature for ionic fluids and existence of spontaneous polarization for a neutral surface for symmetric electrolytes. They can also predict the loss of orientational ordering of anisotropic fluids at a confining interface.

Continuous Symmetries and Exact Solutions to the Vlasov-Maxwell Plasma Models

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Kinetic plasma theory models are based on the Vlasov - Maxwell integro - differential systems of equations. Standard Lie group methods do not allow us to find continuous symmetry transformations of these models. Nevertheless, the symmetries can be deduced from the Lie groups of symmetry of the infinite system of partial differential equations for the moments of particles distribution functions, as it was done in [1] in the case of spatially one dimensional electron-positron plasma.
Another way to find the kinetic symmetries is provided by the use of the finite systems of partial differential equations in the cold plasma limit of the kinetic theory. Traditional Lie group methods can be used in full in this case. Standard Maple programs allow us to find symmetries in this limit. Since the manifold of the cold plasma limit solutions is the most symmetric sub-manifold of the general kinetic theory solutions, we can expect to deduce from the symmetries of this sub-manifold the full continuous symmetry group of the considered kinetic model. This program was realized for many different collision less non relativistic plasma models, the results were presented in [2] for the particular case of spatially three dimensional electron-positron plasma.
Further symmetry extensions are possible if we weaken the integrability conditions on the particle distribution functions as it is described in [3].
The method [1] as well as many other possibilities of finding the kinetic theory symmetries are presented in a review book [4], the recent results of [2] and [3] essentially supplement this review.

[1] V.B. Taranov, Problems of Atomic Science and Technology **1**, 63 (2007).
[2] V.B. Taranov, 7th Int. Conf. Electronics and Applied Physics, October 19-22, Kyiv, Ukraine, 188 (2011).
[3] V.B. Taranov, SIGMA **4**, 006 (2008).
http://www.emis.de/journals/SIGMA/2008/006/
[4] Y.N. Grigoriev, N.H. Ibragimov, V.F. Kovalev, S.V. Meleshko, Lecture Notes in Physics, **806**, Springer, Dordrecht (2010).

Part 5

Nuclear Physics

10 October, 14:30 - 17:50

Three-cluster microscopic description of ^{11}B and ^{11}C

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Mirror nuclei ^{11}B and ^{11}C are very interesting objects for experimental and theoretical investigations. They have a large number of bound states (ten in ^{11}B and eight in ^{11}C), which is quite unusual for nuclei of p-shell. Besides, both of them have well-defined set of resonance states formed by two and three-cluster continuum. The latter have not been investigated thoroughly.

We present investigation of structure of bound and resonance states in ^{11}B and ^{11}C within the framework of three-cluster microscopic method. For this aim we use two models designed to study (i) three-cluster continuum and (ii) binary reactions with polarizability of the interacting fragments (clusters). Detail of these models can be found in Refs. [1] and [2]. We selected three-cluster configurations $\alpha + \alpha +^3 H$ and $\alpha + \alpha +^3 He$ as a dominant structure in nuclei ^{11}B and ^{11}C. These configurations allow us to consider binary channels $^7Li + \alpha$ and $^7Be + \alpha$ respectively. Besides, these configurations allow for a realistic description of ^7Li and ^7Be nuclei as two-cluster system $\alpha +^3 H$ and $\alpha +^3 He$ respectively.

Both models make use the square integrable bases to expand wave functions of three-cluster configuration and implement matrix form of the Schrödinger equation with correct boundary conditions. First method [1] employs the Hyperspherical Harmonic oscillator functions while the second method [2] involves both Gaussian and Oscillator basis functions.

We calculate spectrum of the bound states and for each state we determine its size and shape. Monopole and quadrupole transitions between bound states are investigated. Phase shifts of $^7Li + \alpha$ and $^7Be + \alpha$ are determined and parameter of resonance states are obtained. Role of polarization of nuclei ^7Li and ^7Be on parameters bound and resonance states are studied in detail.

We also investigate continuous spectrum above the threshold of ^{11}B and ^{11}C disintegration on three independent clusters and determine resonances embedded into three-cluster continuum. Total and partial widths of the resonances are calculated and dominant channels for decay of three-cluster resonances are revealed.

[1] V. Vasilevsky, A. V. Nesterov, F. Arickx, and J. Broeckhove. Phys. Rev. C, 63, 034606, 2001.

[2] V. S. Vasilevsky, F. Arickx, J. Broeckhove, and T. P. Kovalenko. Nucl. Phys. A, 824, 37, 2009.

How strange can be strange quark matter in a strong magnetic field?

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Strange quark matter can be formed as a result of the deconfinement phase transition in the core of a neutron star, where the density can reach the values of about several times nuclear matter saturation density. We consider the case of a magnetar being a strongly magnetized neutron star in which core the magnetic field strength can be as large as 10^{20} G. Strange quark matter is studied within the framework of the MIT bag model under charge neutrality and beta equilibrium conditions. It is shown that the strangeness content of strange quark matter begins rapidly to decrease in the fields $H \sim (3-4)\cdot 10^{19}$ G so that the population of s quarks becomes practically negligible in the fields $H \sim 10^{20}$ G. However, in such strong magnetic fields one should take into account the effects of the pressure anisotropy [1, 2]. It is shown that the longitudinal (along the magnetic field) pressure vanishes in the critical field being close to 10^{18} G from above, resulting in the longitudinal instability of strange quark matter. The appearance of such instability sets the upper bound on the magnetic field strength which can be reached in the interior of a neutron star with the quark core. As a consequence, the strangeness content of a magnetar quark core remains practically the same as for a quark core of a moderately magnetized neutron star.

[1] A.A. Isayev, J. Yang, Physics Letters B **707**, 163 (2012).
[2] A.A. Isayev, J. Yang, Physical Review C **84**, 065802 (2011).

Unusual manifestations of the Pauli principle in scattering of atomic nuclei

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We studied the effect of the Pauli exclusion principle on collisions between light atomic nuclei and on the formation of continuum wave function of nuclear systems composed of clusters within a microscopic cluster model. Mainly, different three-cluster models fall into two groups: macroscopic and microscopic. In macroscopic models clusters are considered to be structureless particles and cluster-cluster interactions are approximated by some local potentials which are fitted to reproduce relevant data on the cluster-cluster systems. As for the Pauli exclusion principle, it is usually simulated with an additional repulsive potential between clusters. However, the choice of such a repulsive potential is quite ambiguous and within this approximation a complete and accurate exclusion of the forbidden states is not ensured. Furthermore, macroscopic three-cluster model rests on the assumption that cluster-cluster interactions are not affected by the presence of the third cluster, but this is by no means always the case. Moreover, the elimination of the Pauli-forbidden states does not exhaust all exchange effects. Essential part of such effects is directly relevant to the eigenvalues of the antisymmetrization operator. The latter eigenvalues are not identical and determine the realization probability of the corresponding Pauli-allowed basis states in the wave function of the cluster system. Involvement of the eigenvalues of the antisymmetrization operator in the Schrodinger equation leads to changing the relative kinetic energy as clusters approach each other. Consequently, clusters are shown to experience an effective repulsion or attraction arising from the kinetic energy operator modified by the Pauli principle. Such an effective interaction substantially affects the dynamics of the cluster-cluster interaction and can, on occasion, produce resonance behavior of the scattering phase or even a bound state in compound nuclear system. The largest eigenvalues correspond to those basis states that are dominant in the discrete-spectrum states of the binary cluster system and in continuum states of small above-threshold energy. Also we observed that the probability of the presence of a cluster configuration in the lowest basis function for a binary cluster system is proportional to the eigenvalue of the isolated configuration. We studied the $^3\mathrm{H}+n+n$ configuration of the $^5\mathrm{H}$ nucleus and 3α configuration of $^{12}\mathrm{C}$ nucleus within a fully microscopic three-cluster model. We have shown that an asymptotic behavior of the three-cluster wave function in the continuum consistent with the requirements of the Pauli principle corresponds rather to subsequent decay

of the three-cluster system than to the so-called "democratic"or direct decay. In particular, the structure of the Pauli-allowed states of the ^{5}H nucleus was revealed to correspond to the subsequent decay $^5\mathrm{H} \rightarrow n + ^4\mathrm{H} \rightarrow n + n + ^3\mathrm{H}$, while excited states of ^{12}C predominantly decay via $^8\mathrm{Be} + \alpha$ intermediate stage. Hence, the eigenvalues of the Pauli-allowed states contain a wealth of information on a compound system composed of clusters. Meanwhile, the eigenvalues, along with corresponding Pauli-allowed states, depend only on the assumed internal cluster functions, not on the cluster- cluster potential, etc. Analysis of the structure of the eigenfunctions of the antisymmetrizer and behavior of its eigenvalues has never been performed for three-cluster systems, although we believe that it could help to establish some important laws that govern a three-cluster decay of nuclei composed of s-clusters.

Problem of the δ-interaction effectiveness in quantum systems

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Modeling of short-range interactions by delta-shape quasipotentials is used in different parts of quantum physics starting from works of Bethe, Peierls and Fermi. In particular, most widely used approaches are Breit quasirelativistic potentials between electrons and positrons, zero-range forces in Skornyakov-Ter-Martirosyan approximation in nuclear three-nucleon problems, Fermi pseudopotential ideology in solid-state physics, Skyrme effective nuclear forces, Gross-Pitaevskii equation for condensation processes in Bose-gases. The last three approaches can be explained either using the perturbation theory, or with a one-body mean-field approximation that considerably simplifies the corresponding physical problems.

We consider the conception of δ-potentials outside the perturbation theory and outside the mean-field approximation for many-particle systems taking sufficient account of main correlation effects. Our investigation is based on different approaches: exact consideration of the two-particle problem with a superposition of δ-potentials and standard smooth potentials in bound-state and scattering problems, the use of generalized functions sequences for modeling of pointwise two- and three-particle potentials in problems with two, three or more particles, systematic use of appropriate correlation factors for asymptotic estimates of spectra, variational calculations in problems with two, three or more particles with δ-potentials modeled with sequences of generalized functions. All investigations were made for different space dimensionalities.

General conclusions of consistent analysis of δ-potentials can be summarized as follows: in spaces with $D \geq 2$ dimensions the repulsive δ-potentials (Fermi pseudopotentials) are ineffective and make zero contribution to the shift of energy spectra and scattering. They do not change wave functions for standard potentials everywhere except one deleted point where the potential is localized. For attractive δ-potentials the system will always collapse and the renormalization procedure is necessary on a two-particle level in order to give all physical characteristics some finite non-zero values. Repulsive three-body δ-potentials in three-dimensional space even in accurate approach can not prevent the collapse due to attractive two-body δ-potential. Only in spaces with $D < 2$ δ-potentials produce finite values of physical characteristics and as widely known can be used as reasonable simplified models. On the other hand, in three-dimensional space the Skyrme forces and Gross-Pitaevskii equation can be treated as phenomenological models only.

Rare B-meson decay $\bar{B}^0_d \to \bar{K}^{*0}\,\mu^+\,\mu^-$ and contribution of vector resonances

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We study the flavor-changing neutral current B-meson decay $\bar{B}^0_d \to \bar{K}^{*0}\,(\to K^-\pi^+)\,\mu^+\,\mu^-$ [1,2]. This rare decay is currently under intensive experimental and theoretical investigations because it may give information on 'new physics' beyond the Standard model. The emphasis in our study is placed on accurate treatment of the contribution from the processes $\bar{B}^0_d \to \bar{K}^{*0}(\to K^-\,\pi^+)\,V$ with intermediate vector resonances $V = \rho(770)$, $\omega(782)$, $\phi(1020)$, J/ψ, $\psi(2S)$, ... decaying into $\mu^+\,\mu^-$ pair. The fully differential angular distribution is studied. The dilepton invariant-mass dependence of the branching ratio, longitudinal polarization fraction of $\bar{K}^{*0}$ meson and forward-backward asymmetry is calculated and compared with experiment. It is shown [2] that inclusion of the intermediate resonances may considerably modify the branching ratio, calculated in the Standard model without resonances, even in the invariant-mass region far from the resonance locations. This conclusion crucially depends on values of the unknown phases of the $B^0 \to K^{*0}\,J/\psi$ and $B^0 \to K^{*0}\,\psi(2S)$ decay amplitudes with zero-helicity. The results can be useful for analyses of current and future experiments aiming at search for new physics phenomena on BaBar, CDF, Belle and LHCb detectors.

[1] Alexander Yu. Korchin, Vladimir A. Kovalchuk, Phys. Rev. D **82**, 034013 (2010).
[2] Alexander Yu. Korchin, Vladimir A. Kovalchuk, arXiv:1205.3683 [hep-ph] (2012).

Nuclear Excitation at Electron Transition

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We considered all stages of the nuclear excitation at electron transition (NEET), induced by x-ray photons. Such x-ray photons first ionize the inner atomic shell, then an electron from any upper shell fills the vacancy and transfers its energy via virtual photons to the nucleus, afterwards there occurs quick relaxation of the atomic electrons accompanied by much more slow nuclear deexcitation. For realization of this resonant effect the atomic and nuclear transitions should be well matched and have the same multipolarity. NEET has been observed in a number of nuclei. Perhaps most accurate NEET measurements have been performed by Kishimoto et al. [1] on the nucleus ^{197}Au, where detuning of the nuclear and electron transition energies amounts only 40 eV. Previously the NEET process was only treated in the second order of the perturbation theory [2] and in the framework of the strict collision theory [3]. For analysis of all NEET stages we developed the modified version of the collision theory, combining equations of standard collision theory and quantum electrodynamics. It allowed us to explain naturally all findings of Kishimoto at al. near the K-absorption edge of x-rays in golden target. Namely, we found that the NEET edge is shifted with respect to the K-absorption edge by 40 eV as well as is much steeper and begins below the K-absorption edge. The photo-induced NEET is also considered in ^{178}Hf as a possible explanation of triggering of the 31-year isomer, declared by Collins et al. [3]. We assumed that the incident x-ray photon ionizes the L_3 shell, an electron from the M_5 orbit fills this vacancy and transfers its energy to ^{178}Hf , which makes then transition from the 16^+ isomeric level to an intermediate level. Branching ratios for the deexcitation transition from the intermediate state, bypassing 16^+ level, is significant if the nucleus in the intermediate state has triaxial shape. Even in this favorite case our estimations for the decay acceleration of 31-year isomer by x-rays are by 3 orders of magnitude lower than the predictions of Collins. Note also that such estimations correlate with more refined experiments of other authors. At the same time, they are much higher than the estimations of Tkalya [4], who adopted the axial shape of ^{178}Hf in all states.

[1] S. Kishimoto et al., Phys. Rev. C:, 74, 031301(R) (2006).
[2] E.V. Tkalya, Phys. Rev. A: 75, 022509 (2007).
[3] A.Ya. Dzyublik, JETP Letters: 93, 489 (2011).
[4] C.B. Colins et al., Rad. Phys. and Chem.: 71, 619 (2004).
[5] E.V. Tkalya, Phys. Rev. C: 68, 064611 (2003).

Spin-triplet anisotropic superfluidity in dense neutron matter with generalized Skyrme interactions in strong magnetic field

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In the framework of generalized non-relativistic Fermi-liquid approach we study phase transitions in spatially uniform dense pure neutron matter from normal to superfluid states with spin-triplet p-wave pairing (similar to anisotropic superfluid phases $^3He\ \ A_1$ and $^3He\ \ A_2$) in steady and homogeneous strong magnetic field H (but $|\mu_n|H \gg E_c < \varepsilon_F(n)$, where μ_n is the magnetic dipole moment of a neutron, E_c is the cutoff energy and $\varepsilon_F(n)$ is the Fermi energy in neutron matter with density of particles n). The previously derived [1] general formulas (valid for arbitrary parametrization of the effective Skyrme interaction in neutron matter) for phase transition (PT) temperatures $T_{C1,2}(n, H)$ (which are functions nonlinear of density n and linear of magnetic field H) are specified here for new generalized BSk21 parametrization of the Skyrme forces [2] (with additional terms dependent on density n) on the interval $0.3n_0 < n < 2.5n_0$, where $n_0 = 0.17$ fm^3 is nuclear density. Our main results are mathematical expressions and figures for PT temperatures in absence of magnetic field, $T_{C0,BSk21}(n) < 0.064MeV$ (at $E_c = 10MeV$), and $T_{C1,2}(n, H)$ in strong magnetic fields (which may approach to $1017G$ or even more as in liquid outer core of magnetars - strongly magnetized neutron stars). These are realistic non-monotone functions of density n (with bell-shaped density profile) for BSk21 parametrization of the Skyrme forces (similar to their non-monotone dependence for generalized BSk18 [3] but contrary to their monotone increase [1] for all previous conventional Skyrme parameterizations).

[1] A.N. Tarasov, Central Europ. J. Phys. 9, 1057 (2011).
[2] S. Goriely, N. Chamel, J.M. Pearson, Phys. Rev. C 82, 035804 (2010).
[3] A.N. Tarasov, J. Phys.: Conf. Ser. (2012) (LT26 Proceedings in press). 1

Bosonic symmetries, solutions and conservation laws for the Dirac equation with nonzero mass

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In addition to the well-known fermionic spin s=1/2 characteristics of the Dirac equation with nonzero mass we consider the bosonic spin s=(1,0) symmetries [1], solutions [2] and conservation laws for this equation. Such hidden property of the Dirac equation has been called by us as the Fermi - Bose duality of this equation. We review also the attempts of other authors in this direction, which were published before our investigations.

For the most simple case of the massless Dirac equation (as well as for the slightly generalized original Maxwell equations) the corresponding results were found by us more then 10 years ago, see e. g. [3] and the references therein. Only putting into consideration of the 64-dimensional extended real Clifford - Dirac (CD) algebra A_{64} (our generalization [1] of standard 16-dimensional CD algebra) enabled us to extend the results on the general case, when the mass in the Dirac equation is nonzero. Note that here 7 gamma matrices obey the anticommutation relations of the CD algebra. Hence, now we start from the 29-dimensional proper extended real CD algebra, which is the subalgebra of A_{64} and is generated by 7 (not 5) gamma matrices. Such proper extended real CD algebra realizes the representation of the algebra of SO(8) group.

The additional elements of the proper extended real CD algebra lead to the additional possibilities. The application of this new mathematical object enabled us to prove the hidden bosonic properties (symmetries, solutions, conservation laws) of the Dirac equation with nonzero mass in both standard and Foldy - Wouthuysen [4] representations. It is the basis for our Fermi - Bose dual consideration of the spinor field.

[1] V.M. Simulik, I.Yu. Krivsky, Phys. Lett. A. **375**, 2479 (2011).
[2] V.M. Simulik at al, arXiv: math-ph, 1112.5712, 24 Dec. 2011, 12 p.
[3] V.M. Simulik, I.Yu. Krivsky, Reports Math. Phys. **50**, 315 (2002).
[4] L. Foldy, S. Wouthuysen, Phys. Rev. **78**, 29 (1950).

Microscopic three-cluster description of states in ^{9}Be and ^{9}B

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The aim of the present paper is to study low-energy spectrum of ^{9}Be and ^{9}B nuclei. It is well-know [1] that only ^{9}Be has one bound state and mirror nuclei ^{9}B has no bound state. Thus all states of ^{9}B and most states in ^{9}Be are resonance states. These states attract large experimental and theoretical attention and efforts. Interest to the resonance states in ^{9}Be and ^{9}B is stimulated by several factors.

Investigation of low-lying states in ^{9}Be is interesting for astrophysical applications and, in particular, for problem of synthesis and abundance of light nuclei in the Universe. Resonance states in ^{9}Be, which reside above three-cluster threshold, determine speed of ^{9}Be synthesis in Supernovae. Capture reaction $\alpha(\alpha\mathrm{n}, \gamma)^9$Be could proceed through a resonance state, provided that there is a big concentration of neutrons inside the Star. This reaction can be followed by the reaction $^9\mathrm{Be}(\alpha,\mathrm{n})^{12}\mathrm{C}$. These two reactions is an alternative way to the three-alpha-particle capture reaction in synthesis of nuclei with A>8.

It is interesting to compare spectra of two mirror nuclei ^{9}Be and ^{9}B. They display effects of the Coulomb interaction. The effects are especially intriguing for the $1/2^+$, $1/2^-$ and $5/2^+$ states. Despite dozens years of investigation of these states in ^{9}B there is no clear picture about their position and properties.

Experimental value the quadrupole momentum of the ^{9}Be ground state is very large [1]. This nucleus is strongly clusterized. The neutron separation energy equals 1.67 MeV. This indicates that the three-cluster configurations α+α+n and α+α+p are dominant one in ^{9}Be and ^{9}B respectively. Nucleus ^{9}Be is of a Borromean type of nuclei, because there are no bound states in two-cluster subsystems α+α and α+n. This nucleus and ^{9}B are very interesting subjects for microscopic and semi-microscopic methods.

To study properties of ^{9}Be and ^{9}B we make use of three-cluster microscopic model which was formulated in [2] and demonstrated its efficiency for investigating set of three-cluster nuclei (see, for instance, [3]).

Our results satisfactory agree with the available experimental data and results of other theoretical investigations.

[1] D. R. Tilley, et al., Nucl. Phys. A **745**, 155 (2004).
[2] V. S. Vasilevsky, et al., Phys. Rev. C, **61**, 034606, (2001).
[3] A. V. Nesterov, et al., Phys. Part. Nucl., **41**, 716, (2010).

Part 6

Nonlinear phenomena

11 October, 9:30-13:00

From Davydov's ideas to some models of nonlinear matematical physics

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A family of nonlinear dynamical models is briefly discussed which have been suggested on the basis of the Davydov idea - the coupling of a quantum quasiparticle (intramolecula excitation or excess electron) with longitudinal distortions of a one-dimensional lattice. The investigation has been focused on the existence of stable localized excitations moving with nonzero velocities. In particular, the self-trapping mechanism resulting in the existence of subsonic Davydov's solitons has been extended to supersonic velocities due to anharmonicity. Besides supersonic self-trapping solitons, several other soliton-stabilized mechanisms have been studied resulting in nonlinear models being interesting objects for mathematical physics. Particularly, these include: (i) the capture of Davydov's soliton by a non-topological supersonic lattice soliton, (ii) the paring of supersonic solitons through Davydov's soliton, (iii) the lowering of the barrier in a double-well on-site potential of a diatomic lattice due to longitudinal distortions of the basic (heavy) sublattice resulting in the existence of two-component topological soliton solutions with a gap in the velocity spectrum, (iv) the capture and transfers of electrons by topological ionic defects across hydrogen-bonded systems (shuttle mechanism), (v) the influence of transversal degrees of freedom on the soliton motion in molecular chains. For finding soliton solutions for these complex systems the steepest-descent method has been developed.

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Stabilizing role of lattice anharmonicity in the bisoliton dynamics

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We show that in anharmonic one-dimensional crystal lattices pairing of electrons or holes in a localized *bisoliton* (called also *bisolectron*) state is possible due to coupling between the charges and the lattice deformation that can overcome the Coulomb repulsion. Such localized soliton-like states appear as ground traveling *singlet* states of two extra electrons (or holes) bound in the potential well created by the local lattice deformation. We show that bisolitons are dynamically stable up to the sound velocities in lattices with cubic or quartic anharmonicities, with both energy and momentum, maintaining finite values also at the sound velocity. We calculate the bisoliton binding energy and critical value of Coulomb repulsion at which the bisoliton becomes unbound and decays into two independent solitons. We estimate these energies for chain parameters that are typical for biological macromolecules and some quasi-one-dimensional conducting systems (polydiacetylene, copper-oxygen chains, platinum chains, polymers, salts of transition metals, etc.) and show that the Coulomb repulsion in such systems is relatively weak as comparing with the binding energy. The results of the analytical study of interacting electrons with account of their Coulomb repulsion in a lattice with *cubic* anharmonicity are compared with the numerical simulations of two electrons in an anharmonic Morse lattice with account of Hubbard electron-electron repulsion. We find qualitative agreement between both approaches for a broad range of parameter values.

Moving excitations in a cation lattice

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Mica muscovite has a very special characteristic, its recording capability. Tracks from particles as muons can be distinguished in the complex decoration, but the only explanation to most of the tracks is localized excitations, called quodons [1]. They move in the cation layer without mass transport along the lattice directions. In a recent experiment an alpha particle has been sent to one side of a muscovite specimen and it has observed the ejection of atoms at the other side of the layer along a lattice line [2].
What makes the two dimensional, hexagonal lattice that form the cation layer so special? We advance the hypothesis that one reason is because it is made out of repulsive cations, potassium ions in muscovite. As a first step to explore the consequence of the hypothesis we study a one-dimensional model of potassium ions and observe that supersonic kinks [3] with a very different range of energies can propagate long distances riding a sea of phonons and crossing with others.

[1] D. Schlößer, K. Kroneberger, M. Schosnig, M., F.M. Russell, K.O. Groeneveld: Search for solitons in solids. Radiation Measurements 23, 209-213, (1994).
[2] F.M. Russell, J.C. Eilbeck, Evidence for moving breathers in a layered crystal insulator at 300K. Europhys. Lett. 78, 1004, 1-5(2007).
[3] Yu. A. Kosevich ,R. Khomeriki, S. Ruffo Supersonic discrete kink-solitons and sinusoidal patterns with magic wave number in anharmonic lattices. Europhys. Lett., 66, 2127 (2004).

O-41

Localized excitations induced in nonlinear complex biological systems by high density green photons

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Nonlinear Dynamics of the Metabolic Process in Cells

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Using the classical tools of nonlinear dynamics, we study the process of self-organization and the appearance of the chaos in the metabolic process in a cell with the help of a mathematical model of the transformation of steroids by a cell Arthrobacter globiformis. We constructed the bifurcation diagrams obtained under a variation of the dissipation of the kinetic membrane potential. The oscillatory modes obtained are classified as regular and strange attractors. We calculated the bifurcations, by which the self-organization and the chaos occur in the system, and the transitions "chaos-order "order-chaos "order-order,"and "chaos-chaos"arise. Feigenbaum's scenarios and the intermittences are found. For some selected modes, the projections of the phase portraits of attractors, Poincaré sections, and Poincaré maps are constructed. The total spectra of Lyapunov indices for the modes under study are calculated. The structural stability of the attractors is demonstrated. For various types of strange attractors, their Lyapunov dimensions, KS-entropies, and "predictability horizons"are calculated. Some conclusions about the structure of the chaos of strange attractors and its influence on the stability of the metabolic process in a cell are drawn. A general scenario of the formation of regular and strange attractors in the given metabolic process in a cell is found. The physical nature of their appearance in the metabolic process is studied.

Transmitting canals of non-symmetrical two-barrier resonance tunnel structure for the electrons in electromagnetic field with arbitrary intensity and frequency

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Expanding into the Fourier range the exact solution of one-dimensional non-stationary Schrödinger equation which describes the system of electrons interacting with electromagnetic field of arbitrary intensity and frequency and transit through the open two-barrier resonance tunnel structure, the resonance and non-resonance transmitting canals are established [1, 2]. In the resonance tunnel structure under study the electronic states, field satellite states and complexes of super positions of main and satellite quasi-stationary states are observed causing the transmitting canals of the nano-structure with different properties depending on the field characteristics.
The influence of geometric parameters of two-barrier resonance tunnel structure at the properties of transmitting canals for the electrons is investigated. These properties would be also observed for the multi-shell resonance tunnel structures, being the basic elements of different nano-devices: quantum cascade detectors, quantum cascade lasers and so on. Therefore, developing the theory of physical processes in open resonance nano-structures placed into the strong high frequency fields, the complex quasi-stationary states, as super positions of electron and field states are to be taken into account.

[1] N.V. Tkach, Yu.A. Seti, JETP Letters **95**, 271 (2012).
[2] M.V. Tkach, Ju.O. Seti, O.M. Voitsekhivska, Ukr. J. Phys. Opt. **13**, 36 (2012).

On soliton stability in elastic-plastic model with dissipation

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The elastic-plastic model with a second order gradient may be used for description the dynamics of formation and propagation of deformations in a bar on a stage of disstrengthening. In this model a yield strength of material depends not only on strength and deformation but on a second order gradient of deformation also[1]. The model is applicable to the different materials such as metals, concrete or geomaterials. If one takes into account a nonlinear behavior for a diagram of material $\sigma(\varepsilon)$, where σ is a strengthening and ε is a deformation, then for a square dependence a nonlinear equation for deviation $\varepsilon^{'}$ of deformation from homogeneous state ε_0 is described by equation [2]

$$\frac{\partial^2 \varepsilon^{'}}{\partial t^2} + \frac{\partial^2}{\partial x^2}(\kappa \varepsilon^{'} - \frac{1}{2} f(\varepsilon^{'})^2 + \delta^2 \frac{\partial^2 \varepsilon^{'}}{\partial x^2}) = 0. \quad (1)$$

Here $\kappa = \frac{d\sigma(\varepsilon_0)}{d\varepsilon}$; δ is a parameter describing inhomogeneity of the internal structure of material; f is a coefficient describing a deviation of a diagram of material from linear dependence. This equation has no a localized one-soliton solution. Only two-soliton solution like a breather may be obtained under the special conditions.
A generalization of Eq.(1) on a case of taking such a natural process as a dissipation into account leads to the next equation

$$\frac{\partial^2 \varepsilon^{'}}{\partial t^2} + \alpha \frac{\partial^2 \varepsilon^{'}}{\partial x \partial t} + \frac{\partial^2}{\partial x^2}(\kappa \varepsilon^{'} - \frac{1}{2} f(\varepsilon^{'})^2 + \delta^2 \frac{\partial^2 \varepsilon^{'}}{\partial x^2}) = 0. \quad (2)$$

Here α is a dissipation (damping) coefficient. The last equation has a localized one-soliton solution. Multi-soliton solutions may also be constructed without special conditions. In this report one-soliton solution for Eq.(2) is obtained in an explicit form and its linear stability under small fluctuations is considered. The conditions on the parameters of solution and parameters of model are obtained under which this solution is stable.

[1] V. Kukudzhanov, J. Phys. IV (France) **8**, 207 (1998).
[2] N.N. Myagkov, Pis'ma v JTP. **25**, 48 (1999)(in Russian).

Regular solitary waves with massless fields as asymptotically flat space-times

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Within the framework of Einstein's theory we study the properties of the family of asymptotically flat space-times with regular invariants of the curvature tensor, which are solitary waves (solitons). The common feature of these space-times is the existence of dynamic domains, which are some three-dimensional areas, moving respect to each other, where the metric tensor of space-time has a nondiagonal form. We consider three variants of models: solitary wave in a vacuum, solitary wave with electromagnetic field, solitary wave with a massless scalar field. The results are compared with the well-known models: field of a black hole (Schwarzschild space-time), field of a black hole with electric charge (Reissner-Nordstrom space-time), field of a black hole with scalar charge (Fisher space-time).

Adsorption on the Surface of a Deformable Body

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According to the classical Langmuir theory of adsorption, the single-valued corresponden between the gas concentration and the surface coverage occurs. It is well known that taking account of attractive lateral interactions between adparticles, under certain conditions, lead to hysteresis-shaped adsorption isotherms. It is worth noting that, as early as in 1938, in [1], Zeldovich based on an idea on a change in properties of the adsorbent surface in adsorption, predicted a hysteresis of adsorption isotherms if the typical time of adsorption and desorption is much less than the relaxation time of the surface.

To verify the Zeldovych prediction and to investigate the possibility of a hysteresis of adsorption isotherms in the absence of lateral interactions between adparticles, in [2], it is proposed a model taking into account variations in adsorption properties of the adsorbent surface in the process of adsorption–desorption of gas particles on it. To this end, each adsorption site is simulated by a one-dimensional linear harmonic oscillator oscillating perpendicular to the surface in a certain adsorption-induced force. Within the framework of the mean-field approximation, we derive a system of two nonlinear differential equations that describe the kinetics of the amount of adsorbed substance and a normal displacement of adsorption sites in localized adsorption. The system contains a new characteristic called a coupling parameter equal to the normalized adsorption-induced activation energy for desorption of an adparticle due to the adsorbent deformation in adsorption.

In the stationary case, it is shown that the system under study can be bistable if the coupling parameter is greater than a critical value and the gas concentration belongs to a certain interval. Thus, not only attractive lateral interactions between adpartciles but also the adsorption-induced deformation of the adsorbent lead to bistability of the system, which confirms the Zeldovych prediction of hysteresis due to retardation of relaxation of the adsorbent surface relative to adsorption processes. The surface coverage kinetics on a deformable surface also essentially differs from the Langmuir one. In the overdamped approximation, in the case where the gas concentration is close to a bifurcation value, variations in adsorption properties of the surface lead to the appearance of a "quasistationary" state of the system.

[1] Ya.B. Zeldovich, Acta Physicoch. URSS. **8**, 527 (1938).
[2] A.S. Usenko, Phys. Scr., **85**, 015601 (2012).

Part 7

Posters

Quantum-mechanical calculation of structure and IR spectrum of $2,3$-di--nytro-methhil-β-D-glucopyranoside

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The IR spectrum of the $2,3$-di-O-nytro-methyl-β-D-glucopyranoside have been measured by room temperature. The analysis of the IR spectrum measured at the room temperature indicates the presence of $H-$bonds. How the H-bonds influence to the structure of the sample? Structural–dynamic models of the molecule of $2,3$-di-O-nytro-methyl-β-D-glucopyranoside and its H-complexes are constructed by density functional method [1] (the functional B3LYP, the basis $6-31\ G(d)$. Their energies, structures, dipole moments, polarizabilities have been calculated. Using the results of the quantum chemistry calculations and the calculations of the IR spectrum of H-complexes of the $2,3$-di-O-nytro-methyl-β-D-glucopyranoside and ethanol the following conclusions can be made. The complexing influence only the geometry of the fragments bordering with the core of the H-complex. The lengths of the bonds $-$ of hydroxyl groups in the transition of the molecules to the complexes are increasing by $0,1$ Å and make up $0,98$ Å . The energies of hydrogen bonds are different: from $7,4$ to 10 kcal/mol (dimers) and from $5,7$ to $10,2$ kcal/mol (complexes with ethanol). The changes of frequencies of valent oscillations of the $O-$ bonds are $108cm^{-1}$ and $216cm^{-1}$, which qualitatively consistent with the obtained data for the energies of hydrogen bonds. The difference of the frequencies of valent oscillations of the $O-H$ bonds at the $H-$complexes with difference at the structure was $110cm^{-1}$. It is possible to held their spectroscopic identification. The results of the modeling allowed to interpret the measured IR spectrum of the $2,3$-di-O-nytro-methyl-β-D-glucopyranoside taking the H-complexes into account.

[1] Frisch J., Trucks G.W., Schlegel H.B. et al., Gaussian03, Revision B.03; Gaussian, Inc., Pittsburgh PA, 2003.

Calculation of structure and vibrational spectra of cyclohexanol

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In a wide range of temperatures infrared absorption spectra of cyclohexanol in the plastic (I) and crystalline (II, III) phases were measured. The measured spectra differ from each other. These differences are due to their belonging to the different polymorphic modifications. In this connection the question about detailed study of polymorphism by quantum theory and vibrational spectroscopy methods and identification of polymorphic modification become more actual problem. By density functional method using the functional B3LYP in the basis $6-31G(d)$ structural-dynamic models of conformers of cyclohexanol molecule and its H-complexes (dimer, trimer, tetramer 1, tetramer 2) were constructed. Energies were minimized, structures were optimized, mechanical and electro - optical parameters, the normal modes frequencies in the harmonic approximation and the intensity distribution in the IR spectra were calculated. On the basis of the analysis of calculated IR spectra of the conformers and the measured spectra their preliminary interpretation was given. The spectral and structural characteristics (frequencies) allowing to distinguish between conformers with different structures were determined. Vibrations which sensitive to the orientation of the hydroxyl group relatively the carbon ring of the molecule were identified. On the basis of the analysis of the structure and spectra simulation results of the H-complexes conclusions about implementation of conformers with the equatorial orientation of the hydroxyl group in the crystalline phases II, III and about implementation of conformers with different orientation in the plastic phase. It was theoretically justified that the crystalline phases II and III are formed by the $H-$complexes representing tetramers of the molecules: in phase II - cyclical, in phase III - chained, like a wave ("wave-like"chain). In the phase III' formation of trimer is possible. Plastic phase probably contains all of the $H-$complexes and its IR spectrum in the $3200-3700cm^{-1}$ has a broad, structureless band. By complexing the geometry of the fragments of the molecule forming the core of the H-complex is changed, the conformation of the "chair"of hydrocarbon ring is retained.

P-03

Nonlinear Nambu-Goldstone waves

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For non-Abelian $O(3)$-invariant Goldstone model, as nice example of the spontaneous breakdown of global symmetry, we show the existence of solitary massless waves: nonlinear analog for Nambu-Goldstone waves. Solitary waves are dark and bright waves on the background of Higgs vacuum condensate and have the high symmetry. The solitary waves must satisfy the famous Kasner constraints ("Kasner sphere") for homogeneous anisotropic cosmological models. For Abelian $O(2)$ Goldstone model, a parametric representation of circle in the rational numbers, the usual Noether currents have fractal structure and the fractionalization of charges. For $O(2)$ and $O(3)$ Goldstone models kink-soliton duality give multisolitary waves, fractal structure of solutions, fractionalization of charges, degeneration of Hamiltonian levels to ground vacuum state in the Goldstone model.

Drift vortices in non-equilibrium magnetized plasmas. A Brownian dynamics study

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First-principle Brownian dynamics simulations are employed to study the formation and properties of vortex structures emerging in non-equilibrium magnetized plasmas on a diffusive time scale. The non-equilibrium state of plasmas is maintained due to the recombination and generation of charges. In simulations performed for 2D- and 3D geometry, we examined the behavior of the Coulomb energy, kinetic energy of drift motion, and the plasma structure. The simulations have demonstrated that, for strong magnetic fields and intensive charge recombination and generation, the magnetized plasmas form steady-state vortex dissipative structures (DS). Direct visual observations of plasma configurations as well as the behavior of the Coulomb energy of the system indicate spatial separation of positive and negative plasma components, which means that the steady plasma state in these DS is far from equilibrium. In the absence of pumping, the relaxation of tA.A. Eremko [2], Y. Natanzon [3]
he DS gives rise to the formation of rotational vortex modes with a high extent of coherency, which slowly decay due to the dissipation present in the system. A simple analysis of solutions of the associated kinetic Smolukhovsky equation with allowance for the magnetic field confirms the possibility of existence of the long-lived vortex states with spatially separated plasma components. We expect that the predicted dissipative and coherent vortex structures could be observed in such physical systems as the electron-hole plasmas in semiconductor, or magnetized space plasmas.

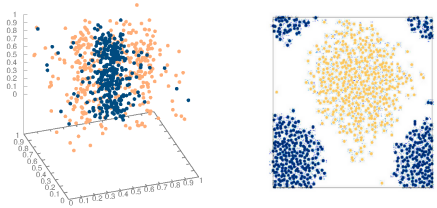

Рис. 7.1: Examples of 3D dissipative (left) and 2D coherent (right) vortex structures emerging in non-equilibrium magnetized plasmas.

Phase-field simulations of eutectic melting

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The phenomenon of contact melting observed in eutectic systems is studied within the framework of phase field theory (PFT). In order to derive the equations describing the dissipative structural dynamics of complex media, PFT exploits the Ginzburg-Landau formalism. To examine the eutectic melting, we employ in the simulations the simplest form for the free energy functional, where the eutectic properties are provided by the chemical miscibility gap of solid components. The computer simulations were carried out for 1D- and 2D binary systems, for the range of parameters typical for real materials, with allowance for heat transfer as well as within the isothermic approach. The simulations have demonstrated that PFT is capable to reproduce the basic features of contact melting observed in experiments. After the short initial stage accompanied by the formation of liquid layer between the solid components, the melting proceeds to a steady state, which depends on the parameters, the phase diagram and the initial state of the system. The results obtained suggest the diffusive nature of contact melting, since the latter is observed within the isothermic approximation.

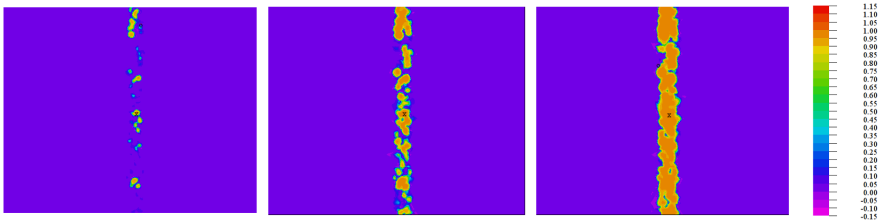

Рис. 7.2: Typical distributions of phase variable during the initial stage of contact melting in a planar binary eutectics for the time points t=0.011 ms (left); 0.012 ms (middle); and 0.013 ms (right).

Transport of magnetized particles in a frozen turbulent electric field

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Transport of particles and energy in plasma is one of the most important problems of controlled nuclear fusion. There is widely used numerical simulations with a large number of particles to study it. However, it is necessary to know basic mechanisms of transport in a turbulent fields to explain results of numerical experiments. For this purpose more tractable models are considered, in particular a model of test-particle motion in a prescribed random fields.
The crucial point of this problem is to establish the relation between Lagrangian correlation function, which is determined along particles trajectories, and Eulerian correlation function, which is determined in a laboratory frame and can be measured in experiments. Some solutions of this problem were found for a small correlation time of turbulent fields, but there is no solution in general case.
The decorrelation trajectory method [1], which is supposed to be capable to deal with a large correlation times has been proposed recently. We applied this method to describe statistical behaviour of particles in a frozen turbulence that characterized by an infinite correlation time. Basic assumptions of this method along with calculated particle dispersion are compared with the results of direct numerical simulation. Other approaches [2,3] to this problem are discussed as well.

[1] M. Vlad, F. Spineanu, J.H. Misguich, and R. Balescu, Phys.Rev. **E 58**, 7359 (1998).
[2] V.I. Zasenko, A.G. Zagorodny, O.M. Chernyak, UJP **56**, 1007 (2011).
[3] J.B. Taylor and B. McNamara, Phys.Fluids **14**, 1492 (1971).

P-07

New insight into the physical nature of the "glacial" phase in triphenyl phosphite

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During the past decade polyamorphic transition between two amorphous states (or two liquids) in triphenyl phosphite, focused considerable attention. As a result of polyamorphic transition a new solid phase denoted as "glacial" phase was observed. However the nature of this "glacial" phase remains controversial. To gain understanding in this subject we havA.A. Eremko [2], Y. Natanzon [3]
e conducted infrared spectroscopy investigation of the structural changes during the glaciation and crystallization processes in triphenyl phosphite. For the first time it was experimentally illustrated that different crystalline modifications can be obtained upon variation of crystal growth conditions. At low temperatures in the vicinity of the glass transition nucleation of the low-temperature (LT) polymorph is favored. This LT phase at the nanometric size comprise the "glacial" phase. Thus the "glacial" phase is a mixed crystallites – supercooled liquid state. We have not found any evidence of polyamorphism in triphenyl phosphite. LT polymorph can be obtained from the "glacial" phase which transforms into crystal phase by heating ("glacial" crystallization). Another high-temperature (HT) polymorph can be obtained from the liquid phase due to direct cooling from room temperature up to 240, 250, or 260 K. Hence the concept of polyamorphism does not apply to the case of TPP, at least.

Mixed exciton-plasmon collective elementary excitations of the Bose-Einstein condensed 2D magnetoexcitons with motional dipole moments

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The collective elementary excitations of the two-dimensional magnetoexcitons in the state of their Bose-Einstein condensation (BEC) with different from zero wave vector $\vec{k}$ and in-plane parallel oriented motional dipole moments are investigated in the Hartree-Fock-Bogoliubov approximation. The breaking of the gauge symmetry is achieved following the Bogoliubov theory of quasiaverages in combination with Keldysh-Kozlov-Kopaev method. The starting Hamiltonian and the Green's functions are determined using the integral two-particle operators instead of single-particle Fermi operators. The infinite chains of equations of motion for the multioperator four and six-particle Green's functions are truncated following the Zubarev method introducing the small parameter of the perturbation theory related with the lowest Landau levels filling factor and with the phase space filling factor. The energy spectrum of the collective elementary excitations consists from mixed exciton-plasmon energy braches, mixed exciton-plasmon quasienergy branches as well as from the optical and acoustical plasmon energy branches. The exciton branches of the spectrum have the gaps related with the negative values of the chemical potential and attractive interaction between the two-dimensional megnetoexcitons with in-plane, parallel oriented motional dipole moments. The slopes of the mixed exciton-plasmon branches are determined by the group veloA.A. Eremko [2], Y. Natanzon [3]
cities of the moving condensed excitons as regards the laboratory reference frame. The acoustical and optical plasmon energy branches are gapless with linear and quadratic dependences correspondingly on the small wave vectors accounted from the condensate wave vector $\vec{k}$ and with saturation dependences in the range of higher wave vectors.

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Mössbauer spectra of ferromagnets in radio-frequency magnetic field

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In numerous experimental papers it was shown that the Mössbauer absorption spectra of soft ferromagnets, exposed to the rf field of circular frequency Ω, consist of equidistant lines spaced by Ω. At low frequencies the absorption spectrum transforms to standard Zeeman sextet and at high frequencies it collapses to single line or doublet.

These observations were explained by the step-wise reversals model [1-4]. Its main assumption is that the magnetization $\mathbf{M}(t)$ of soft ferromagnets exposed to the rf magnetic field, periodically changes its orientation. The magnetic fieA.A. Eremko [2], Y. Natanzon [3]

ld at the nucleus $\mathbf{h}(t)$, being antiparallel to $\mathbf{M}(t)$, repeats such reversals skipping between the values $-\mathbf{h}_0$ and $+\mathbf{h}_0$ with the same period $T = 2\pi/\Omega$. Then each level of the nucleus, subject to the periodic field $\mathbf{h}(t)$, splits into equidistant infinite set of quasi-energies, spaced by $\hbar\Omega$ and the absorption spectrum attributes a fringe structure [1].

If a constant magnetic field is superimposed along the rf external field, the reversals become asymmetric in time and the magnetic field at the nucleus averaged over time is not zero. We have shown that this ensures quasi-Zeeman splitting of the nuclear quasi-levels and corresponding splitting of absorption lines into quasi-Zeeman sextet [2,3]. In addition, the rf field induces in ferromagnets the magnetostrictive vibrations. Combination of both mechanisms allowed us to obtain good fitting of the experimental absorption spectra [2]. We also analyzed transient effects, arising when the period T much exceeds the nuclear lifetime. The field reversal are shown to cause oscillations of the time-dependent absorption cross section of γ-quanta [1] as well as strong flash of the radiation, transmitted through a ferromagnet [4].

At last, the dynamical scattering theory is developed [5], taking into account both the periodical reversals of the magnetic field at the nuclei and magnetostrictive vibrations. It is found that the coherent transmitting gamma wave in the crystal absorbs or emits only couples of the rf photons. As a result, the forward scattering spectra of γ quanta consist of equidistant lines spaced by twice the frequency of the rf field in contrast to the absorption spectra. These findings well correlate with our experimental data [5].

[1] A.Ya. Dzyublik, phys. stat. sol. (b) **194**, 699 (1996).
[2] A.Ya. Dzyublik and V.Yu. Spivak, JETP **84**, 794 (1997).
[3] A.Ya. Dzyublik, et al., JETP Lett. **67**, 61 (1998).

[4] A.Ya. Dzyublik, J. Phys.: Condens. Matter **11**, 3915 (1999).
[5] A.Ya. Dzyublik, et al., Nucl. Phys. and Atomic Energy, **13**, 73 (2012).

Effects of electrostatic field on Davydov's mechanism of charge transport in low-dimensional systems

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We study the dynamics of self-trapped electrons (or holes) in a one-dimensional molecular chain with periodical boundary conditions under the influence of the external electrostatic field, taking into account the interaction of an electron with acoustical phonons. The dependence of the average velocity of such soliton-like solutions on the field magnitude and on the system parameters is calculated. It is shown that the electrosoliton moves in the electrostatic field with acceleration together with the local chain deformation. The initially stationary localized electron in a chain starts moving after some period of rest even in fields weak as compared with the Peierls-Nabarro potential in a discrete chain. We show that the process of electrosoliton acceleration can be controlled by the intensity of the field and extent of the energy dissipation. At some values of the dissipation constant for the given intensity of the field, soliton acceleration vanishes and soliton velocity attains constant value. We also have observed the oscillations in the electrosoliton dynamics due to the influence of the Peierls-Nabarro relief. These oscillations are enhanced at strong values of the dissipation constant when the system is far from being completely integrable.

Weak pulsed electric fields and bacteria respiration

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The theoretical analysis introduces a definite clearness into the comprehension of the mechanisms of the processes defining the reaction of bacteria to the treatment with weak impulse electric fields (IEF) without any damage of cells. The change in the respiratory activity of bacteria P. fluorescens resistant to cyanides while treating impulse electric field had been experimentally found by [1]. The theoretical analysis of the experimental data indicates the change of quantity of active respiratory centers in cells while influencing impulse electric field. Such change bears reverse character. Depending on the state of bacteria the processes of inhibition or restoration of the respiratory centers by impulse electric field can be observed.
A specific feature of the interaction of bacteria and IEF consisted in that the RA of active cultures decreased, whereas the cells with decreased respiratory activity, on the contrary, restored or even increased the. The use of cyanide (silver dicyanide complex) as a respiratory blocker retarding the electron transfer confirmed experimentally the hypothesis about the possibility to activate a respirator center on the application of the external field. This can be realized by the mechanism of nonlinear tunneling of electrons present in the quantum wells formed by some redox pairs of respirator centers. The executed estimates indicate the reversibility of the processes of inhibitory blocking and deblocking of respirator centers on the application of IEF. The dependence of the respiratory reaction on the treatment duration indicates the cumulative character of this effect. It may assume that the regularities, which are observed in experiments with bacteria of a single genus, have a more general character and are applicable to various biological objects undergoing the action of weak electric (electromagnetic) fields. The task of researchers will consist in the selection of such parameters of fields which would allow the deblocking of the transfer of electrons in respirator centers, by rendering the therapeutic effect on living objects.

[1] V.I. Podolska *at all*, Food Biophysics. 2009. **4**, 281.

Molecular dynamics and phase behavior of binary mixtures of stearic acid and cetyltrimethylammonium bromide as studied via Davydov splitting of molecular vibrational modes

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Due to their intriguing properties, such as an ability to spontaneously form various aggregates in dilute aqueous solutions including micelles, bilayers, tubes and vesicles, as well as organized self-assemblied monolayers, mixtures of surfactants of opposite charge, called a catanionic surfactants, cause much interest during the past decades. This interest is connected both with fundamental importance of molecular self-aggregation and with a variety of its industrial applications for encapsulation and controlled delivery processes. Equimolar mixtures of cationic and anionic surfactants were shown to exhibit also peculiar properties in condensed state, both in the bulk or in the self-assembled monolayer, though still little is known regarding the phase behavior of these systems. In this work, we study the temperature-induced phase transitions in equimolar mixture of stearic acid ($C_{17}H_{35}COOH$, SA) and cetyltrimethylammonium bromide ($C_{19}H_{42}NBr$, CTAB) with particular attention to the complex formation and its effect on the enhanced temperature stability of the material compared to pure acid or CTAB. The temperatures of the transitions were determined by differential scanning calorimetry (DSC, Perkin-Elmer DSC7), and FTIR spectroscopy was used to investigate the molecular dynamics and structure of the complex. FTIR spectra (3804000 cm^{-1}) were collected at variable temperature from 300 to 450 K with IFS-88 Bruker spectrometer (64 scans, spectral resolution 2 cm^1). DSC analysis shows a set of successive phase transitions in the solid state along with a much higher melting temperature of the SA-CTAB mixture than that of the pure acid. This is a clear indication of the strong interaction in the mixture and suggests a formation of molecular complex. This is confirmed by FTIR spectroscopy. The FTIR absorption spectra of SA-CTAB show that the carbonyl band (1710 cm^1) of pure acid disappear in the spectra of the mixture that proves the attachment of CTAB head group to the OH group of the acid and formation of SA-CTAB complex. As it has been established in our earlier works [1-3], Davydov splitting of molecular vibrational modes of long-chain aliphatic compounds may be used to evaluate alkyl chain ordering in different crystal phases. From the

temperature dependence of the Davydov splitting of CH_2 rocking (720730 cm^1) and scissoring (14601470 cm^1) absorption bands, the changes of alkyl chains packing in the various phases of the complex are inferred. The possible molecular mechanisms of successive phase transitions are discussed with regard to interaction between the acid surfactant and the CTA^+ counterion.

[1] S.P Makarenko, G.A Puchkovska, E.N Kotelnikova, S.K Filatov. Journal of Molecular Structure, 704 (1-3), 25 (2004).
[2] G. Puchkovska, S. Makarenko, V. Danchuk, A. Kravchuk. Journal of Molecular Structure, 744-747, 53 (2005).
[3] T. Bezrodna, G. Puchkovska, V. Styopkin, J. Baran, M. Drozd, V. Danchuk, A. Kravchuk. Journal of Molecular Structure, 973 (1-3), 47 (2010).

Localized states at a plane defect layer with nonlinear properties

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The research carried out in the present work is connected with a rather new actual direction in modern theoretical physics, the theory of nonlinear waves and solitons in solid state physics. From the viewpoint of technological applications, the largest attention is focused on multilayered or modulated structures of various types. For instance, these are multilayered magnetic systems, multilayered crystals with multiatomic unit cells, and others. In nonlinear optics, layered and modulated media are used in fiber systems, optical delay lines, etc.
In the framework of the quasiclassical approach, we investigate the soliton states localized near a plane defect layer (point defect) which has nonlinear properties, for different signs of nonlinearity and for different characters of the interaction between elementary excitations in the system and the defect layer. The quantum interpretation of these nonlinear localized modes in terms of a large number of bound states of elementary excitations is proposed. The regions of existence are determined and the properties of such states depending on the character of interaction of elementary excitations with one another and with the defect are studied.

[1] Y. Kivshar and G. Agrawal, *Optical Solitons: From Fibers to Photonic Crystals* (Academic, New York, 2003).
[2] H.S. Eisenberg, Y. Silberberg, R. Morandotti, A.R. Boyd, and J.S. Aitchison, Phys. Rev. Lett. **81**, 3383 (1998).
[3] I.V. Gerasimchuk and A.S. Kovalev, J. Phys.: Condens. Matter **13**, L885 (2001).
[4] Kai Li, P.G. Kevrekidis, Boris A. Malomed, and D.J. Frantzeskakis, Phys. Rev. E **84**, 056609 (2011).

Adsorption of polymer chains at penetrable interfaces

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The localization of polymer chains at interfaces is of great interest from both theoretical and technological standpoints because of its various applications. Penetrable interfaces reside in structured surfaces or in layered environments which can be formed in microphase separated block-copolymers, liquid crystalline or lipid systems. The understanding of polymers in environments of multiple interfaces can lead to novel applications for selection and recognition of polymer properties. In the adsorbed state, conformations of localized chains are the result of the interplay between adsorption energy, entropy reduction because confinement in the adsorbed state, and the excluded volume repulsion between the monomers. Taking into account excluded volume effects is most important to understand the physics of real polymers close to surfaces or interfaces.

In the present work we study the exact solutions for the problem of localization of real polymer chains with excluded volume interaction in the system of two attractive transparent interfaces in the framework of mean-field approximation. An array of interfaces on nanostructured surfaces can be an example of such a system. At first, we introduce the model for the case of a single penetrable interface and after we present the exact solution for the case of two penetrable interfaces. The total number of monomers in such systems is exactly calculated. The saturation values for the total number of monomers are found. We obtain a non-monotonic behaviour for the dependence of the number of adsorbed monomers on the distance between interfaces. Such a behaviour of the saturation density of polymers leads to the two-phase character of the dependence of free energy as a function of the number of adsorbed monomers. We find also the exact expressions for the total energy of the system and for the saturation value of the energy. At the saturation point, we find that the force acting between the attractive interfaces is strictly attractive and monotonously decaying towards zero for increasing interface distance.

[1] Jens-Uwe Sommer and Alexander Blumen, Phys. Rev. Lett. **79**, 439 (1997).
[2] J. Martin, M. Vazquez, M. Hernandez-Velez, and C. Mijangos, Nanotechnology **19**, 175304 (2008).
[3] P.G. de Gennes, *Scaling Concepts in Polymer Physics* (Cornell University Press, Ithaca and London, 1979).

Localization of an optical beam at two nonlinear lightguides in anharmonic medium

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The investigations of the localization character of nonlinear waves in periodic layered and modulated systems have always been a focus of attention in nonlinear waves dynamics. The possibility of the spatial localization of light flux in a few neighboring waveguides perpendicularly to the direction of its propagation is well-known. Earlier the propagation of nonlinear wave flux along two coupled parallel plane waveguides in anharmonic medium (nonlinear Kerr medium) was described. Assuming that the waveguides and environment differ in refractive indexes, the discrete nonlinear dynamical equations describing the field amplitudes in waveguides were obtained. The possibility of localization of nonlinear wave flux in one waveguide was demonstrated. Later the nonlinear Kerr terms were taken into account only in the waveguides because of the smallness of average field amplitude in the wide regions for a weak waveguides coupling.
The goal of the present work was the investigation of the more general case, viz., the stationary localized states of light fluxes propagating along a system of two identical parallel plane nonlinear optical waveguides in the medium with Kerr nonlinearity in the framework of the nonlinear Schrödinger equation. The solution for an optical flux localized perpendicularly to the direction of its propagation was analytically derived. It was shown that all of the parameters (the total "intensity the total energy) of the system are found exactly from the microscopic description of the problem.

[1] I.V. Gerasimchuk and A.S. Kovalev, JETP Letters **85**, 488 (2007) [Pis'ma v ZhETF **85**, 594 (2007)].
[2] I.V. Gerasimchuk and A.S. Kovalev, J. Phys.: Condens. Matter **13**, L885 (2001).
[3] Y. Kivshar and G. Agrawal, *Optical Solitons: From Fibers to Photonic Crystals* (Academic, New York, 2003).
[4] Kai Li, P.G. Kevrekidis, Boris A. Malomed, and D.J. Frantzeskakis, Phys. Rev. E **84**, 056609 (2011).

Classical Structures of Charges in the Confining Potential of the Uniform Cylindrical Background. Equilibrium States

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It is of a general and practical interest to understand what shapes of external confining potentials would be responsible and preferable ones in the formation of ordered low-dimensional structures of charges at the given direction(s) on a finite length scale. Confinements of an axial symmetry, quite desirable in this context, were experimentally fabricated in the studies of ionic and electronic cold plasmas trapped in limited space volumes by static electric and magnetic fields, and structures of any dimensionality, but somewhat disordered in interparticle spacings, were realized under such conditions [1]. Peculiarities and salient features of confining potentials play also the key role in the self-organization of electronic structures in semiconductor nanosystems [2] and on the surface of liquid He [3] at low temperatures.
In this work we deal with a model electrostatic confinement originated from the uniform cylindrical background of the length $2L$, radius R and the whole charge eN. Confining potential for carriers with a charge $-e$ can be written by the quadrature

$$V_{conf}(x,\rho) = -\left(\frac{e^2}{\varepsilon} n_{1D}\right) \frac{4}{R} \int\limits_0^\infty \frac{dk}{k^2} J_1(kR) J_0(k\rho) \left\{F(k(L+x)) + F(k(L-x))\right\},$$

where $F(k(L \pm x)) = \exp\left(-\frac{k}{2}|L \pm x|\right) \sinh\left(\frac{k}{2}(L \pm x)\right)$ and $n_{1D} = N/2L$ is the linear density of a background, ε is a dielectric constant of a medium. Carriers interact one with another by the Colomb law. Ionic power of a system follows from the balance between the charging parameters of carriers and background. Priority is given to neutral systems. A wide range of initial parameters was covered in calculations.
Results, based on the classical approach, include, in particular, the $1D$-structures with high level of linear ordering under the condition $L/NR \cong 1$, $2D$-structures which appear as linear zigzag or planar structures in longitudinal or relatively flat systems respectively, inner $2D$-associations of charges in $3D$-cluster systems of finite length. In coclusion, we assure that the model confinement proposed stands a good chance to be exploited usefully in quantum treatments to charge systems refered in [1-3].

[1] D.H.E. Dubin, T.M. O'Neil, Rev. Mod. Phys. **71**, 87 (1999).
[2] G. Piacente, G. Q. Hai, and F. M. Peeters, Phys. Rev. B **81**, 024108 (2010).
[3] Yu.Z. Kovdrya, Fizika Nizkih Temperatur **2**9, 107 (2003).

Oscillations of Plasmon Linewidth in Metal Nanoparticle Embedded in Various Dielectric Media

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The investigation of the plasmon linewidth in metal nanoparticle has attracted much attention in recent years [1,2]. It is known that the damping of the plasmon are an essential parameter, since it contains the information about the character of interactions in the system, in particular, about the lifetime of the surface plasmon. The important aspect of the plasmon linewidth is its oscillations depending on the nanoparticle radius [3,4].
For the description of the plasmon linewidth behavior, we used the kinetic approach [4-6]. In present work we demonstrate how the damping of the surface plasmon is changed as a function of the particle radius, shape, and the light frequency. The main attention is paid to the electron surface-scattering contribution to the plasmon decay. We predict the surface plasmon linewidth oscillations with varying the dielectric constant ϵ_m of the media in whose a spheroidal metal nanoparticle can be embedded. The oscillations are well pronounced for nanoparticles with the small radii and disappeared for ones with a larger radii. The magnitude of these oscillations is the greater the smaller particle is and enhances markedly with ϵ_m.
The resonance plasmon damping in the *oblate* metal nanoparticle was found stronger along the spheroid revolution axis than the one across this axis. For the *prolate* metal nanoparticle, on the contrary, the damping along the revolution axis was weaker than the one across this axis. All calculations of the plasmon linewidth are illustrated by the example of the Au and Ag nanoparticles with different radii. The results obtained in the kinetic approach are compared with the known ones from other models.

[1] M. Hu, C. Novo, A. Funston et al., J. Mater. Chem. **18**, 1949 (2008).
[2] Z. Yuan, S. Gao, Surf. Sci. **602**, 406 (2008).
[3] G. Weick, R.A. Molina, D. Weinmann and R.A. Jalabert, Phys. Rev. B, **72**, 115410 (2005).
[4] N.I. Grigorchuk and P.M. Tomchuk, Phys. Rev. B **84**, 0854488 (2011).
[5] N.I. Grigorchuk and P.M. Tomchuk, Phys. Rev. B **80**, 155456 (2009).
[6] P.M. Tomchuk and N.I. Grigorchuk, Phys. Rev. B **73**, 155423 (2006).

Processes of Photothermal and Photoacoustic Energy Conversion in Inhomogeneous Semiconductor Structures: Theory and modeling

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This paper presents the results of energy conversion processes investigation in inhomogeneous semiconductor materials under their irradiation by short laser pulse. The methods that are based on Photothermal and Photoacoustic (PA) phenomena successfully applied in various fields of modern material research [1]. However, processes occurring at energy transformation "*light- thermal-sound*"are not fully understood. This especially regards to PA phenomena study in a heterogeneous media. For description of these processes it should be taken into account a number of different factors, ranging from the characteristics of light absorption in a heterogeneous environment to the effect of boundaries influence on generated non-stationary heat distribution and transformation of chaotic (*thermal*) in phased (*acoustic*) oscillations of atoms in a photo-excited heterogeneous environment.
We consider the formation of non-stationary temperature distribution in heterogeneous semiconductor materials at their irradiation by short laser pulse. A mathematical model of PA conversion in such structures based on the equations of thermoelasticity [2] has been developed. The proposed model gives the possibility to analyse the dispersion dependence of elastic waves excited by pulse laser irradiation in confined inhomogeneous semiconductor structures.

[1] Progress in Photothermal and Photoacoustic Science and Technology: Vol. **4**, Semiconductors and Electronic Materials, Eds. Mandelis A., Hess P., SPIE Optical Engineering Press, Bellingham, 2000
[2] W. Nowacki, Thermoelasticity, PWN, Pergamon Press, (1986).

Two-dimensional solitons in binary mixtures of Bose-condensates

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One of most prominent nonlinear structures that can emerge in attractive Bose-Einstein condensate is a bright soliton. It is well known, that two- and three-dimensional bright solitons are unstable with respect to collapse if their number of particles is overcritical. The simple idea to arrest the collapse is to use a mixture of atoms with repulsive inter-component interaction. It turns out, that soliton-soliton pairs in trapless two-component BEC are unstable - the more powerful component collapses [1].
Mixtures of Bose-Einstein condensates (BECs) are interacting quantum systems of macroscopic scale which exhibit rich physics not accessible in a single-component degenerate quantum gas. They open up intriguing possibilities for a number of important physical applications, including quantum simulation, quantum interferometry, and precision measurements. Experimentally, multi-component BECs are generated as mixtures of atoms in different hyperfine states or by simultaneously trapping different atomic species.
In present work we study solitonic structure in mixtures of trapped BECs. We consider different geometries of "disk-shaped"trapping potential including parabolic trap and toroidal trap. We perform detailed theoretical analysis of nonlinear structures, including investigation of steady-states and stability analysis. Different scenarios of unstable evolution have been observed. It was found that stable solutions exist. As the result of our investigations we perform region of the stability of soliton-soliton pairs [3].

[1] A.I. Yakimenko, O.O. Prikhodko, and S.I. Vilchinskyi Phys. Rev. E, Vol.82, 016605 (2010)
[2] A.I. Yakimenko, Yu.A. Zalinzyak, V.M. Lashkin Phys. Rev. A, Vol. 79, 043629 (2009)
[3] A.I. Yakimenko, K.O. Shchebetovska, S.I. Vilchinskii, and M. Weyrauch, Phys. Rev. A, Vol. 85, 053640 (2012)

The model of a polymorphic macromolecule bendability.

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Usually, to describe the bending of chain macromolecules a model of elastic rod considering the deformations both homogeneous and small - a model of WLC (Worm like chain) is used. However, for polymorphic macromolecules such as DNA the data where the deformation is neither homogeneous nor small is known. In such cases to describe the deformation one must take into account features of polymorphic macromolecules: anharmonicity of the energy of deformation, the correlation between the different components of deformations, in other words - nonlinear effects. This paper presents a study of DNA bending as a polymorphic macromolecule, taking into account the interrelation between the elastic components and the possibility of conformational transformations.

We have previously shown that a bistable conformation of a fragment of DNA chain may induce a significant bend of the double helix [1]. The conformation-induced deformation in DNA chain is realized under the transition between the bistable states and under decrease in stiffness by 45%. Such conditions may be fulfilled for a specific sites of DNA chain.

In this paper we consider the effect of including of interrelations between different elastic degrees of freedom of macromolecules on the conformation-induced mechanism of DNA deformation. Introducing the interrelation between the torsional and bending components the conformation-induced bending of DNA fragment is considered. The results show that conformational mechanism of deformation is favorable with a decrease in stiffness by 19% only. An additional inclusion of the interrelation of double helix stretching and twisting and further reduction of stiffness over the noted above values leads to greater advantage of the conformationally-induced in over the elastic deformation mechanism.

Using the model of conformational induced bending with interrelations between components the amount of significant bends (kinks) realized in the closed fragment of the double helix have been calculated. The obtained results are qualitatively and quantitatively consistent with the results of numerical experiments [2] and show the reality of the proposed mechanism.

[1] P.P. Kanevska, S.N. Volkov, Ukr.J.Phys. **51**, 1003 (2006)
[2] F. Lankas, R. Lavery, J.H. Maddocks, Structure **14**, 1527 (2006).

Cooperative control of transient characteristics of an open quantum system with fluctuating energies

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A microscopic model of cooperative control of the process of irreversible binding between the ligand and the receptor molecules in solution is developed. The model is based on a concept of an open quantum system coupled to a condensed medium and experiencing both the relaxation transitions between different quantum states and thermal fluctuations of the energy levels [1]. Analytical expressions for the amplitudes and integral yields of transient states of a system averaged over equilibrium vibrations in the medium and stationary random shifts of system's energy levels are derived. It is shown that in the presence of irreversible kinetic stage, even in the case of linear non-cooperative binding of ligand to receptor, the dependence of transient amplitudes on ligand concentration demonstrates an essential property of system's cooperativity. Such a property becomes most apparent in the Hill's coefficient that characterizes the log odds to favor of the process of system's control in respect to the concentration changes. It is obtained that Hill's coefficient is reduced to some value which is less than and generally nonintegral in comparison with the corresponding integer initially characterized the system. It is found that this effect is influenced by the degree of system heterogeneity as well as by the intensity of fluctuations in the system. It is also observed that both these phenomena are acting in a consensus providing for the less cooperativity in the more heterogeneous systems as well in the systems exhibiting the more high-intensive energy fluctuations.

[1] V.I. Teslenko, O.L. Kapitanchuk, Ukr. J. Phys. **57**(5), 573 (2012).

New Trends in Physics of Nonlinear Group Syncronisms in the Phonon Field of Condenced Matter

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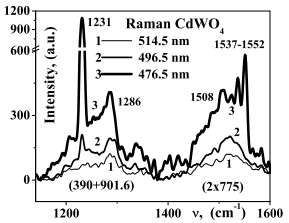
When agreeing group velocities, except the broad band of nonlinear wave interaction it becomes possible the energy concentration (EC) of waves of different frequencies in one wave. We have developed the concept of vectorial group and multiple non-critical in frequency and angle phase-matchings (PM) [1]. The concept is based on consideration of general properties of the PM surface, built in the coordinates of frequencies and angles, and also the analysis of singular lines and points where broadband and wide-angle PMs can occur. At critical values of ω_{LCR} the PM surface contracts to a point. Neighborhood of this critical point corresponds to a triple non-critical PM in frequency ω_S and two angles.There is a deep analogy between the critical points of nonlinear interaction of waves and the critical points of phase transitions (PT), which opens a fundamentally new direction for studying the nonlinear wave nature of PT. In the resonant phonon field nonlinear susceptibility increase greatly, but because of the nonlinearly-induced dispersion of medium the nonlinear detuning of wave-vectors Δk_{NL} appear. In this case, the optimal conditions for nonlinear wave conversion can take place when Δk_{NL} is compensated by a linear wave detuning Δk_L. The manifestation of the vectorial group PMs in the vibrational [9]l0.46



spectroscopy of overtones and combination tones is observed for the first time. In the Raman spectra of the crystal $CdWO_4$ excited by 514.5 nm were observed broad bands of overtone 2x775 $cm^{-1}$and the overall tone of 390+901.6 cm^{-1}, as shown in figure. At the short-wavelength excitation (496.5 and 476.5 nm) in the middle parts of the bands occur sharp peaks at 1231 and 1509, 1537 $cm^{-1}$with half-widths

$\delta = 6-8$ cm^{-1}. Their intensities are 5-9 times higher than the intensity of the bands at 514.5 nm. The appearance of sharp lines at critical values of ω_{LCR} and other characteristics clearly point to EC within the phonon branches, which proves the important role of nonlinear interactions in the excitation dynamics of condensed matter.

[1] V.I. Zadorozhnii, N.E. Kornienko et al., Functional materials, **12**, 91 (2005).

The regular pattern formation in ferromagnetic films under influence of spin-polarized current

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Process of the saturation of a thin isotropic ferromagnetic film in transverse direction by strong spin-polarized current is studied theoretically. It is shown that the critical current of saturation J_c increases with the film thickness increasing: quadratically for thin films and linearly for thick ones (comparing with the exchange length). We show that appearance of stable *square vortex-antivortex superlattices* (crystals) precedes the saturation. Spatial period of the superlattice weakly decreases with the current increasing. With the current decreasing the transition from crystal phase into "fluid" phase occurs, where the long-range order in the superlattice is destroyed but the short-range order is preserved. The micromagnetic simulations confirms our analytical results with a high accuracy.

The phenomenon of vortex-antivortex superlattices formation was studied in detail both numerically [1,2] and analytically [2]. Our numerical study was based on computer micromagnetic simulations using OOMMF code [3] and our analytical approach was based on the discrete Landau-Lifshitz-Slonczewski equation [4]. The linear analysis of stability of the saturated state enable us to obtain the value of the saturation current J_c as function of material parameters and the film thickness. The weakly nonlinear analysis proves the possibility of stable square vortex-antivortex superlattices in the pre-saturated regime. The transition from crystal phase into fluid phase was studied only numerically. We show that parameter Λ (it describes the mismatch between spacer and ferromagnet resistance in the pillar structure) does not influence the saturation current J_c, and influence of Λ on the dynamics of the vortex-antivortex superlattice is very weak. But the critical current J_{fc} of the transition fluid phase – crystal phase, and consequently the current range of the crystal phase $[J_{fc}, J_c]$, depends on the parameter Λ significantly: the crystal region vanishes when $\Lambda \to 1$ and it is constant for $\Lambda \gg 1$.

[1] O.M. Volkov, V.P. Kravchuk, D.D. Sheka, Yu. Gaididei, Phys. Rev. B **84**, 052404 (2011).
[2] Yu. Gaididei, O.M. Volkov, V.P. Kravchuk, D.D. Sheka, arXiv:1206.4125 (2012).
[3] The Object Oriented MicroMagnetic Framework, version 1.2α4, http://math.nist.gov/oommf/
[4] J.C. Slonczewski, J. Magn. Magn. Mater. **159**, L1 (1996).

Modelling of nerve signal transmission in chemical synapse

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In our paper we considered the process of transmission of nerve impulses in chemical synapse. Assuming that the process of transmission of chemical neurotransmitter in synaptic cleft is slower than the interaction with receptors in postsynaptic membrane, we have constructed a model of signal transmission in synaptic cleft. In our work we found changes of quantity of activated receptors on the postsynaptic membrane in time, which play an important role in the transmission of nerve signals. Also, the transmission of a series of nerve impulses through chemical synapse was considered in this model.

Observation and study of new physical phenomena in layered ferroelastic crystals ($Cs_2Bi_2I_9$)

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Ferroelastics is a peculiar new class of crystalline solids in which the spontaneous strain of a crystal lattice is appeared relatively of initial one as a consequence of structure phase transition from more symmetrical (paraelastic) phase into less symmetrical (ferroelastic) phase. One of ferroelastics is the $Cs_3Bi_2I_9$ layered semiconductor that have high anisotropy of chemical bonding: a strong ion-covalent bonding in the separate layer sandwich and a weak Van der Waals interaction between the neighbouring sandwiches. The review report deals with the experimental and theoretical studies of new phenomena registered. The following problems were solved towards this purpose:

- A nontraditional for the layered substances temperature shift of the fundamental absorption edge $Eg(T)$ of $Cs_3Bi_2I_9$ was observed. It is shown that this shift is described very well by the Varshni formula.
- The transition region from 150 to 220 K was registered. It is shown that this region may be identified as the heterophase structure region where ferroelastic and paraelastic phases coexist.
- A change of exciton-phonon interaction from strong to a weak as temperature decreases was found on the same sample. The effect is explained on the basis of a model that takes into account the reconstruction of the crystal lattice from layered to non-layered one. The temperature value $T^* = 150K$ may be considered as characteristic one below of which the crystal loses the nature of layered substance.
- Raman spectra of $Cs_3Bi_2I_9$ were studied in heating regime over temperature range 5-300 K but any soft mode or softening of modes were not observed. The interpretation of Raman spectra is given.
- The structure phase transition in $Cs_3Bi_2I_9$ at $T_c = 220$ K was registered. It is shown that this transition is the first order transition which is close to the second order one.

- A new giant thermodynamical optical effect near the ferroelastic phase transition point was found and explained on the base of Landau-Khalatnikov theory.

[1] F.V.Motsnyi, M.V.Vuychik, O.M.Smolanka and E.Yu.Peresh //Functional Materials, vol.13 (2005).
[2] F.V.Motsnyi, O.M.Smolanka, V.I.Sugakov and E.Yu.Peresh //Solid State Communs., vol.137 (2006).
[3] F.V.Motsnyi, O.M.Smolanka, E.Yu.Peresh, S.V.Virko and V.G.Dorogan //Physica: Condensed Matter., vol.B 403 (2008).

Shake-up processes in the magneto-photoluminescence spectra of the two-dimensional hole gas and acceptor-bound trions

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The aim of our paper is to explain the unusual shake-up process observed experimentally [1] in the magneto-photoluminescence spectra of the two-dimensional hole gas (2DHG) with the participation of the acceptor-bound positive trions AX^+. Side by side with the emission lines of the free exciton (X), and trions (X^+), as well as of AX^+ the shake-up (SU) emission line named as AX^+SU in the presence of the magnetic field perpendicular to the layer and varying in the interval up till 23 T was revealed. The unusual behavior of the AX^+SU line consists in the fact that at small magnetic fields it is situated on the lower energy side of the AX^+ line at the distance comparable with the cyclotron energy but at increasing magnetic fields it shifts gradually his position to the higher energy side of the line AX^+. Being the Stokes-type shake-up emission line it transforms continuously into the anti-Stokes shake-up line. Such behavior was observed in the presence of a strong electric field caused inside the structure of the asymmetric GaAs/GaAlAs quantum well by the one sided doping. Our explanation is based on the investigation of the energy spectrum of the Landau quantization of the heavy holes taking into account the Rashba spin-orbit coupling, the nonparabolic dispersion law and the third order chirality terms following the Refs. [2, 3]. It was shown that the lowest Landau levels are characterized by two-component spinor-type wave functions with the quantum numbers $m - 5/2$ and $m + 1/2$ at $m \geq 3$. Their dependences on the magnetic field strength are nonmonotonous. For example, the pair of the Landau levels with $m = 3$ and $m = 4$ are changing their relative positions on the energy scale. So in some regions of the magnetic fields the lower is the level with $m = 3$, whereas in another regions the lower is the level with $m = 4$. The transitions between the levels $m = 3$ and $m = 4$ in the first case needs to absorb energy, whereas in the second case to emit it. We suppose that in the AX^+ complex there are bound three heavy holes on the Landau level with $m = 3$ because they have the smallest radii of Landau quantizations and are closely bound in the frame of A^-+e+3h*structure.Thesesuppositionspermittoexplaintheexperimentaldata.*

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[1] J. Jadczak et al., J. Phys.: Conf. Ser. **210**, 012043 (2010).

[2] T. Hakioğlu et al., J. Phys.: Cond. Matt. **23**, 345405 (2011).
[3] S.A. Moskalenko et al., Solid State Comm. **151**, 1690 (2011).

P-27

On time as a quantum observable, canonically conjugated to energy, in quantum mechanics and in quantum field theory

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During long time, beginning from the publication by Pauli on non-relativistic quantum mechanics near 90 years ago, it is known that time cannot be represented by self-adjoint linear operator. It follows from semi-bounded-ness of continuous energy spectra (usually they are bounded by zero from the bottom). The foundation of the author works on the problem of time is the Naimark theorem which says that the non-orthogonal spectral development $E(\lambda)$ of any hermitian operator H belongs to the Karleman type, so it can be approximated by the sequence of self-adjoint operators, the spectral developments of which weekly converge to the spectral development $E(\lambda)$ of the operator H. And this non-orthogonal spectral development is unique for the maximal hermitian operator. Namely with the help of this theorem it was shown in the author works that time can be introduced as a quantum observable, canonically conjugated to energy, for the physical systems with continuous spectra of energy. And it was shown that for such systems time operator is usually maximal hermitian operator. Also in those works it was solved the question about the measure (or the weight function) of averaging over time in the agreement with the averaging procedures and known principles of quantum mechanics. Then it was cleared that for systems with the discrete energy spectra time is a quantum observable, canonically conjugated to energy and time operator is quasi-self-adjoint operator. Moreover, there it was also shown that for maximal hermitian operator and self-adjoint operator energy it is fulfilled the uncertainty relation $E\Delta t \geq \hbar/2$, which has the same sense as for the uncertainty relation for coordinate-impulse. And in other author works there results were generalized for the quantum field theory (quantum electrodynamics, the Klein-Gordon equation and the Dirak equation). Then the results of time analysis for quantum and nuclear processes, founded on the application of time as a quantum observable, are presented.

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Generalization of Polynomial Invariants of Torus Knots

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The interplay between knot theory and physics manifests itself in various ways. The special attention is given to the investigation of polynomial invariants of knots and links. The Jones polynomials, for example, are widely used in the quantum field theory. The Alexander knot polynomials can be generalized to the HOMFLY knot polynomials [1, 2]. Since the Jones, Alexander and HOMFLY knot polynomials provide the most important characteristics of knots and links, their generalization is believed to be helpful for describing of knot-like structures.

[1] A.M. Gavrilik, A.M. Pavlyuk, Ukr. J. Phys. **55**, 129 (2010); arXiv:0912.4674v2 [math-ph].
[2] A.M. Gavrilik, A.M. Pavlyuk, Ukr. J. Phys. **56**, 680 (2011); arXiv:1107.5516v1 [math-ph].

Relaxation time in bistable tunneling system

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In recent years, the investigation of nonlinear systems far from equilibrium under the influence of stochastic forces (or noises) has received great attention. It is known that noise forces near the points of instability can induce new phenomena such as noise-induce transition, slowing down of the dynamics and others. The important aspect of the dynamical behavior of the system is the fluctuation decay depending on some parameters of noise and system [1,2].
In the present work we studied noise effects on the process of tunneling of electrons through a double-barrier nanostructure. For the description of tunneling process we used the model given in [3,4]. The considered system is nonlinear nonequilibrium system having a bistability behavior. Dynamics of the system is defined by the time dependence of the intensity of electron flow $I(t)$ passing through the system.
Under the influence of noise, the system can transit from one stable state to the other one. This transition can be characterized by the relaxation time which determines the critical slowing down when passing through a barrier. The relaxation time is defined by the expression

$$T = \int_0^\infty C(s)/C(0)ds\,,$$

where $C(s) = \lim_{t\to\infty}\langle\delta I(t+s)\delta I(t)\rangle - \langle I\rangle_{st}^2$ is the correlation function of the system and is the fluctuation of the intensity flow. Based on the numerical computation and simulation results, it was found that for some values of , the relaxation time is enhanced and its maximum value increases with increasing the correlation time of the noise. From these data it can be concluded that a noise-induced transition is presented.

[1] J.M. Sancho et al.,Phys. Rev. A **32**, 3639 (1985).
[2] J. Casademunt et al., Phys. Rev. A **35**, 5183 (1987).
[3] A.S. Davydov, V.N. Ermakov, Physica D, **28**, 168 (1987).
[4] E.A. Ponezha, Ukr. J. Phys. **55**, 243 (2010).

Global optimisation study of the protein off-lattice model with applied external force

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We report the results of a systematic global-optimisation search for the global minima of the off-lattice 46-bead 3-color protein model [1] pulled apart by an applied external force. In our study, the applied force is assumed to be constant and is applied to the end atoms of the model protein, and the basin-hopping method [2] is used to perform exploration of the underlying energy landscape of the model protein. Both the original wild-type and the Gō -like [3] models were studied. The motivation for studying this problem stems from the recent advances in single-molecule experiments in which a biological molecule (e.g. a protein) is stretched apart by the atomic force microscope or laser optical tweezers[4], providing a convenient technique for studying the protein folding process from another perspective. The model studied is widely used as a toy model for studying protein folding and therefore is a natural starting point for modelling a protein pulling experiment, before switching to more realistic and complicated models. Our results show that, as the applied force increases, there is a sequence of structural transitions during which the protein arms discontinuously unfold in the one-by-one fashion, indicating the presence of hysteresis in the present system. Our results qualitatively corroborate the findings from other groups [5].

[1] Honeycutt, J. D. and Thirumalai, D. Biopolymers 32 (1992), 695.
[2] Wales, D. J. and Doye, J. P. K. J. Phys. Chem. A 101 (1997), 5111.
[3] Nymeyer, H., Garcia, A. E., and Onuchic, J. N. Proc. Natl. Acad. Sci. USA 95 (1998), 5921.
[4] Ritort, F. J. Phys. Condensed Matter. 18 (2006), R531.
[5] Imparato, A., Luccioli, S., and Torcini, A. Progress of Theoretical Physics Supplement 184 (2010), 339.

Uncertainty of coordinates distribution of inhomogeneous particles under the influence of gravity

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As it has been shown earlier, the distribution of distances between two bounded particles with different shapes and dimensions in viscous medium is determined unambiguously by their interaction potential and macroscopic parameters as a result of dissipative processes [1]. Do other variants of analogical uncertainties exist? Let us consider the model system consisting of multitude analogical inhomogeneous non spherical free particles. Let their averaged density be equal to the density of the medium. Therefore their movement along gravity field can be described as:

$$m\ddot{x} + h\dot{x} = A(t), (1)$$

where m is a particle mass; h is friction coefficient depending on its orientation toward the movement direction; x is coordinate of mass centrum of a particle; A(t) is fluctuation force. Let us integrate (1) with respect to x. According to the T-symmetry and the law of equipartition, we will obtain:

$$(\bar{h_1} - \bar{h_2}) \int_{x_1}^{x_2} \bar{\dot{x}} dx = 2 \int_{x_1}^{x_2} \bar{A} dx, (2)$$

where $\bar{h_1}$ and $\bar{h_2}$ are correspondingly averaged friction coefficients for a particle which moves from point x_1 to point x_2 and back; $\bar{\dot{x}}$ is averaged velocity of the particle. Under the certain conditions the particles are oriented in gravity field and $\bar{h_1} \neq \bar{h_2}$. In the case of averaging with the respect to the ensemble of all particles, $\bar{\dot{x}} = 0$. From (2) it means that the probability of the particle location in point x_1 $P(x_1)$ is equal to $P(x_2)$. But in the case of averaging with the respect to the ensemble of the particles which move from one point to the other being not returned to previous location during this transition, $\bar{\dot{x}} \neq 0$, and therefore in some real systems $\frac{P(x_1)}{P(x_2)} \approx e$. Thus, there the coordinates distribution is uncertain.

[1] O.I. Pundyak, Uzhg. Uni. Sci. Herald, Phys.: **21**, 186-190 (2001).

Deterministic and chaotic vortex dynamics in magnetic nanodots

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One of the effective ways of the magnetic vortex core reversal in a nanodisk can be realized under the action of ac magnetic field. Recently, the resonance switching of the vortex polarity under the action of ac perpendicular field was found numerically [1,2]: when the field frequencies are tuned to the eigenfrequencies of radial spin-wave modes, the threshold field amplitudes required for vortex-core switching are an order of magnitude smaller than those of static perpendicular fields. In this work we study such a switching in details both numerically and analytically. Different switching regimes are found when changing the field intensity H_0 and its frequency f. In particular, the vortex polarity demonstrates a chaotical dynamics with $1/f$ spectrum in a wide range of H_0 and f. We analyze the chaotic behavior of the system by means of autocorrelation functions, phase trajectories and Poincaré maps. We predict also a deterministic oscillations with resonance at the $f_0/3$ frequency which leads to polarity switching. We study the controlled vortex polarity switching under the influence of a short wave train: the controlled unidirectional switching takes place for low field amplitudes.
We present an analytical approach to describe simulations data using the vortex core model [3]. Our model is in a very good agreement with results of numerical simulations.

[1] R. Wang, X. Dong, Appl. Phys. Lett., **100**, 082402 (2012).
[2] M.-W. Yoo, J. Lee, S.-K. Kim, Appl. Phys. Lett. **100**, 172413 (2012).
[3] Y. Gaididei, T. Kamppeter, F. G. Mertens, A. R. Bishop, Phys. Rev. B **61**, 9449 (2000).

Theoretical Modelling of Liquid Crystals Filled with Ferroic Nanoparticles

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Liquid crystal colloids display a richer set of properties than conventional colloidal systems [1]. Of these, ferroelectric and ferromagnetic liquid crystal colloids have been the subject of considerable recent work [2-5]. Here the colloidal particles are so small that the suspensions seem optically identical to pure liquid crystal, but nevertheless the dielectric response is strongly enhanced, even at low colloidal concentrations, and the liquid crystalline clearing temperature can even be raised by several degrees Kelvin. Our theoretical model of the dielectric properties of a ferroelectric LC nanosuspension supposes that the suspension may as a first approximation be considered as a complex homogeneous dielectric ceramic. The suspension then consists of an anisotropic matrix with a very low concentration ($< 1\%$ by volume) of impurity particles, possessing both shape and dielectric anisotropy, a permanent electric polarization and strong liquid-crystal director anchoring on the particle surface. We calculate the effect of doping a liquid crystal with ferroelectric impurities on the Frederiks transition. The theory takes account of inclusion shape, dielectric susceptibility, and local field effects. Our calculations [4] suggest, in qualitative agreement with experiment, that doping a nematic liquid crystal with ferroelectric particles can in some cases significantly shift the electric Frederiks threshold field. We also study the switching properties of a ferronematic in a nematic liquid crystal cell subject to an external magnetic field and homeotropic boundary conditions at the cell and particle walls. We find different regimes, depending on the strength of the anchoring interaction between the director and the ferroparticle orientation. For low anchoring strengths, there is an inverse Frederiks (IF) effect [5]. If the dimensionless temperature scale in the problem is low, then high magnetic fields can cause magnetic segregation. Coupling of the segregation order parameter to the director distortion can change the IF transition into a first order transition, leading to bistability [5].

[1] H. Stark, Phys. Rep., **351**, 387 (2001).
[2] Yu. Reznikov et al., Appl. Phys. Lett., **82**, 1917 (2003).
[3] G. Cook et al., Optics Express, **16**,4015 (2008).
[4] S. Shelestiuk et al., Phys. Rev. E, **83**, 041705 (2011).
[5] V.I. Zadorozhnii et al., SIAM J.Appl.Math, **68**, 1688 (2008).

Research of kink's movement changes after interface passing

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The aim of this research is to find out and to analyse changes in kink's dynamics while its passing through the interface between two phases. This interface divides two DNA sequences coming one after another. Crank-Nicolson method is used to solve the sine-Gordon eqution numericaly. As a result of numerical experiments it was found that drastic changes of the mode of the nonlinear wave take place, which is caused by passing through the interface and due to characteristics of each of these sequences [1]. Depending on kink's energy density, which is different for each type of homogeneous DNA sequence there are some possible alternatives for further mode of movement after reaching the interface: reflection from the interface, passing through the interface with velocity decrease and passing through the interface with velocity increase. Furthermore kink- antikink transition is shown in case of reflection from interface.

[1] L.V. Yakushevich, L.A. Krasnobaeva, A.V. Shapovalov, N.R. Quintero Biophysics - Vol. **50**, No. **3**, 2005, pp. 404-409.

Theory of superfluidity of rarefied gases of composite bosons

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The microscopic theory of superfluidity of a rarefied Bose gas consisting of an alkali metal atoms is constructed. We take into account that such atoms generally do not act as bosons. The ground state wave function is chosen as a coherent state analogous to the state proposed by Keldysh for an electron-hole gas. This wave function contains an unknown order parameter $\Phi(\mathbf{r}_1, \mathbf{r}_2)$, for which a nonlinear nonlocal integro-differential equation is obtained. This equation is a generalization of the Gross-Pitaevskij equation for bosons with internal degrees of freedom.
The question about electric polarization of electrically neutral homogeneous and inhomogeneous superfluid systems is researched. The problem is to solve the equation for the order parameter $\Phi(\mathbf{r}_1, \mathbf{r}_2)$. In the homogeneous case we consider the possibility of spontaneous polarization in the superfluid systems. It is shown that this phenomenon has a threshold type (the interaction energy of bosons must exceed the distance between the ground and excited states). In a spatially inhomogeneous system the dipole moment appears inevitably (without any threshold) and has the form $\mathbf{P} = Cena_B^5 \partial n/\partial \mathbf{R}$, where n is the density of particles, a_B is the Bohr radius, C is of the order of unity.
Also we consider two methods of microscopical description of systems consisting of composite bosons: in terms of the two-particle order parameter $\Phi(\mathbf{r}_1, \mathbf{r}_2)$ [1, 2] and in terms of the set of one-particle order parameters $\Psi_i(\mathbf{R})$ [3, 4]. It is determined that these two approaches are substantially different. If we apply the second method to composite bosons we completely lose the exchange interaction effects. Moreover, even neglecting the exchange interaction we can adequately describe the system with the set of one-particle order parameters $\Psi_i(\mathbf{R})$ only when we take into account all internal states of the particles. In this case it is necessary to solve an infinite set of equations for $\Psi_i(\mathbf{R})$.

[1] S.I. Shevchenko, A.S. Rukin, JETP Letters **90**, 42 (2009).
[2] S.I. Shevchenko, A.S. Rukin, Low Temp. Phys. **36**, 146 (2010).
[3] D.N. Zubarev, Inhomogeneous statistical thermodynamics, Moscow, Nauka (1971).
[4] Yu.M. Poluektov, Low Temp. Phys. **37**, 986 (2011).

Control of the current through a molecular junction by a locally applied electric potential

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Current control in molecule-size devices is one of the most significant problems of molecular electronics. It is shown [1] that an electron current through a linear molecule embedded between the attached electrodes, is formed by two mechanisms of electron transfer. They are a sequential hopping and a distant tunneling (superexchange). Efficiency of each mechanism is determined by molecular orbitals' energies as well as by molecular length [2]. Present work demonstrates some results concerning a control of the molecular junction's conductance by additional electrode field applied to internal part of a molecule.

The object of interest is the system "electrode–molecule–electrode" where the molecule consists of terminal sites and a linear bridge of N identical sites between them. All the sites are characterized by a good localization of extra electron. However, the probability of a transferred electron to occupy the bridge remains rather low (because its energy on the internal sites is too high). An additional electrode (gate) is placed near an internal part of the molecule. The gate field can increase or decrease energy of the bridge's molecular orbitals changing thereby a barrier for distant tunneling as well as an electron hopping between the bridge's sites and the respective terminal sites. To study the influence of the energy alteration on the efficiency of electron transfer mechanisms and conductance of the molecule we have used nonequilibrium density matrix theory. The calculations show that at a given voltage bias the dependence of an interelectrode current strength on a gate potential is near exponential. At the same time, the shape of the current-voltage dependence of the system under consideration stays almost unaffected by the gate potential because the shape is formed mainly by both terminal site-electrode interactions and voltage bias factors [3]. From the results obtained one can conclude that the gate electrode placed near a low-occupied part of a molecule (in a system "electrode–molecule–electrode") can be used to control a molecular conductance without change of the features of current-voltage characteristic.

[1] E.G. Petrov, Ya.R. Zelinskyy, V. May, and P. Hänggi, J. Chem. Phys. **127**, 084709 (2007).
[2] E.G. Petrov, Ye.V. Shevchenko, and V. May, Chem. Phys. **288**, 269 (2003).
[3] E.G. Petrov, Ye.V. Shevchenko, and V.I. Teslenko, Mol. Cryst. Liq. Cryst. **467**, 59 (2007).

Fluxon dynamics in the long quasi-one-dimensional Josephson junction with impurities

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The fluxon (magnetic flux quantum in the dielectric layer of Josephson junction) dynamics in a long quasi-one-dimensional Josephson junction with presence of time-independent bias is studied. Fluxons in the junctions can be represented as solitary waves which are the solutions of the two-dimensional sine-Gordon equation on the superconducting condensate wave function phase difference [1]. In our model the junction width is substantially less than its length but is the order of Josephson penetration length λ_J. The presence of the dissipation and the inhomogeneities of different shape (point, line and rectangular) and size is considered. The dependence of the threshold bias current [2] on the junction width is found both analytically with the help of the kinematical considerations and numerically. The retrapping current value decreases with the junction width because it is easier for the quasi-one-dimesional fluxon to pass through an inhomogeneity as compared to the one-dimensional case. Good agreement between the kinematic approximation and numerical results appears for small and intermediate junction width (several λ_J) but not for the large width. It can be explained by the fact that the kinematic arguments are based on the assumption of the absolute rigidity of the fluxon shape in the perpendicular direction but it is clear that for the large width spatial deformations of the fluxon shape start to play an important role. It is shown that after the propagation through the the inhomogeneity fluxon receives the additional mode of oscillation of the wave front (shape waves) with the amplitude that depends on the dissipation properties of the junction.

[1] A. Barone, G. Paterno, Physics and Applications of the Josephson effect, A Wiley-Interscience Publication, New York (1982).
[2] D.W. McLaughlin, A.C. Scott, Phys. Rev. A **18**, 1652 (1978).

Phenomenon of "relativistic" approximation in dynamics of quasi-particles

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The general dynamical properties of free quasi-particles are analyzed [1]. Analyzed also the conditions under which the description of the dynamic properties of the quasi-particles is almost identical with those of real relativistic particles. The problem of the relation of quantum and classical methods of describing the quasi-particles in the case of the excited states of crystals is considered. Basic principles of construction of dynamic properties of classic type for quasi-particles at excitation of matter with the structure of solids (crystals) are analyzed. The results of analysis were demonstrated on the example of electronic excitations of crystals in the simplest case, when other effects are neglected (phonons, defects, high density of excitations, which requires the account of interactions between them, the response of lattice to excitations [2], and so forth). The response of lattice to excitation and influence of the external fields on dynamical properties of quasi-particles were considered in [3]. It was shown that such excitations are described in three ways simultaneously. First is quantum, which gives description of the examined excitations in terms of wave functions and eigenvalues of energy. The second method is classic. It arises out from the quantum method and is formulated in relation to wave impulse. Description of quasi-particle in terms of the second method can be named a wave classic type description. The third method which is derived from the second also a description of the classical type, but in relation to the other impulse – mechanical. In approximations used here (plane wave in a phase, nearest neighbors and cubic grate) the third method of description practically coincides with the known dynamic description of free relativistic particle. This (third or second classical) description makes it possible to interpret the experimental data in terms of the usual relativistic dynamics, if the considered system allows the use of the considered approximations.

[1] Suprun A.D., Shmeleva L.V., The bulletin of the Kiev university. Series phys., 14, 7 (2012) (in Ukrainian).
[2] Suprun A.D., Razumova M. A. The bulletin of the Kiev university. Series phys.-math. sciences, 3, 554 (2006) (in Ukrainian).
[3] Suprun A. D., Dynamic properties of single-electron non-linear excitation of the crystals, Kyiv university", Kyiv (2008), 151 p. (in Ukrainian).

Magnetic susceptibilities of dense superfluid neutron matter with generalized Skyrme forces and spin-triplet pairing at zero temperature

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Magnetic properties of dense superfluid neutron matter (relevant to physics of neutron star cores) at subnuclear and supranuclear densities (in the range $0.5n_0 < n < 3.0n_0$, where $n_0 = 0.17fm^3$ is saturation nuclear density) with the so-called generalized Skyrme effective forces BSk18 [1] and BSk19, BSk20, BSk21 [2] (containing additional unconventional density-dependent terms) and with spin-triplet p-wave pairing in the presence of a strong magnetic field are studied within the framework of non-relativistic generalized Fermi-liquid theory [3,4]. Upper limit for the density range of neutron matter is restricted by the magnitude $3.0n_0$ in order to avoid account of relativistic corrections growing with density. The obtained earlier general formula [5] (valid for arbitrary parametrization of the Skyrme forces) for magnetic susceptibility of superfluid neutron matter at zero temperature is specified here for the BSk18 and BSk19-BSk21 parameterizations of the Skyrme interaction. As it is known all previous conventional Skyrme interactions predict spin instabilities in normal (nonsuperfluid) neutron matter beyond the saturation nuclear density. At the same time we have obtained that for the model of superfluid neutron matter with new generalized BSk18 and BSk19-BSk21 parameterizations such phase transition to ferromagnetic state does not occur neither at subnuclear nor at supranuclear densities, i.e., the paramagnetic susceptibilities of neutron matter for BSk18-BSk21 parameterizations are not divergent, but for BSk18-BSk20 they are non-monotone functions of density which attain maximum in the supranuclear range $1.0n_0 < n < 3.0n_0$, and for BSk21 force paramagnetic susceptibility is monotonically increasing function in this range of densities. Thus, the high-density ferromagnetic instability is removed in neutron matter with new generalized Skyrme forces BSk18 and BSk19-BSk21 not only in normal but also in superfluid state with spin-triplet pairing.

[1] N. Chamel, S. Goriely, J.M. Pearson, Phys. Rev. C 80, 065804 (2009).
[2] S. Goriely, N. Chamel, J.M. Pearson, Phys. Rev. C 82, 035804 (2010).
[3] A.I. Akhiezer, V.V. Krasil'nikov, S.V. Peletminskii, A.A. Yatsenko, Phys. Rep. 245, 1 (1994).
[4] A.N. Tarasov, AIP Conf. Proc. 850, 109 (2006).
[5] A.N. Tarasov, Ukrainian J. Phys. 55, N5, 644 (2010).

On the strong influence of boundaries on the bulk microstructure of an interacting Bose gas. The Gross–Pitaevskii and Bogolyubov approaches

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In the framework of the Gross–Pitaevskii and Bogolyubov approaches, we have considered the interacting Bose gas in a one-dimensional bounded domain and have found two different dispersion laws for phonons. One law coincides with the well-known Bogolyubov one $\hbar\omega(k) \approx \sqrt{\left(\frac{\hbar^2 k^2}{2m}\right)^2 + qn\nu(k)\frac{\hbar^2 k^2}{m}}$ with $q = 1$. The second law is new and is described by the same formula with $q = 1/2$. The new solution corresponds to a less value of the ground-state energy. Therefore, namely this solution should be realized in nature.

Two-state hard-core Bose-Hubbard model: Bose-Einstein condensation in excited band and non-ergodic contribution

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The Bose-Hubbard model is widely used for description of ultracold atoms in optical lattices as well as the dynamics of protons on the metal surface. Such a model with two local states and the particle hopping in the excited band only in the hard-core boson (HCB) limit was analyzed in our previous works [1,2] considering the Bose-Einstein (BE) condensation in this system in the MFA and the RPA. Unlike the common HCB model, the order of the phase transition into the BE condensate state can change from the second order to the first one (related to BE condensation of "holes", while the second order transition leads mainly to the "particle" BE condensation). In the regime of fixed concentration of bosons it corresponds to the phase separation on the normal phase and the phase with the BE condensate. The non-ergodic contribution to the particle momentum distribution is on a par with the ergodic one in the superfluid phase near the tricritical point so the formalism of two-time Green's functions becomes insufficient in this case.
Hence we propose here a unified description of both thermodynamic (phase diagrams) and dynamic (single-particle excitation spectrum, spectral density and momentum distribution) characteristics of the system by means of the temperature Green's function approach considering the correction up to the one sum over wave vector for the grand canonical potential of the system which provides improved expressions for occupations of states. Related changes of the system behaviour are analyzed and compared with our previous results.

[1] I.V. Stasyuk, O.V. Velychko, Condens. Matter Phys., **14** (2011) 13004.
[2] I.V. Stasyuk, O.V. Velychko, Theor. Math. Phys., **168** (2011) 1347.

Fermi-Davydov splitting and many phonon effects in IR spectra of crystals with the strong H-bonds

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The investigation of the vibrational spectra of hydrogen bonded systems in condensed phases is important topic in physics, chemistry and biology. The hydrogen bonded molecular crystals are very convenient objects for such studied since the translation symmetry noticebly simplifies the vibrational problem as well as it helps to clarify the role of anharmonic interactions involved in the phenomenon. However even for simple crystals in which the unit cell contains only one hydrogen bond and considered as good model systems the anharmonic effects are very important. One of them is the phenomena of Fermi resonance (FR). Its influence on the shape band of vibrations was studied an enough detaily (see for example [1] and references herein). However there exist many crystals having several identical hydrogen bonds which are differently oriented. Therefore, as the dipole moments are oriented along the H-bonds one can expect of displaying of the Davydov splitting (DS) effect for H-bond bands in addition to traditional enough complex structure which arises because of strong coupling H-bond vibrations with the lattice phonons [1,2]. Mixing of all these effects FR, DS and many phonon processes, which are due to the strong coupling between high frequency ν-OH and low frequency vibrations (lattice phonons) gives rise to very complicated shape band of vibrations in the region H-bond of crystals. In this communication we consider the effect of discussed above three factors on the absorption shape of band of the H-bond vibration (it was first studied in [2]) and analyze the change of absorption spectrum, its polarization features and ratio between intensities of Fermi-Davydov components on the example of H- and D-adipic acid crystals. Taking into account enough full information, obtained in our ab-initio calculations, about low- and high-frequency region of spectrum, and by varying the coupling constant it was possible to fit the principal theoretical maxima and explain the features of the experimental spectrum of H- and D-adipic acid crystals in the region of hydrogen bond vibrations for two orthogonal polarizations. The variation of spectrum with change of electric field orientation relatively to the crystal axises is theoretically studied too.

[1] H. Ratajczak, A.M. Yaremko, Chem. Phys. Letters, **314**, 122 (1999).
[2] A.M. Yaremko, H. Ratajczak, et all, Chem. Phys. **306**, 57 (2004).

Generalized Stillinger–David potential

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The improved version of the polarizational Stillinger–David potential for intermolecular interaction in water is proposed in the work [1]. The clear and consecutive algorithm for the construction of a function describing the oxygen-hydrogen interaction in water molecule is formulated. The new approach for the modeling of the screening function, responsible for the cutting of charge-dipole interaction on small scales, is developed. For the correct description of the long-range asymptote of the intermolecular potential the bare Stillinger–David potential is completed by the interaction between oxygen dipole moments. Besides, the polarizational part of the bare Stillinger–David potential is completed by a term taking into account the deformation of oxygen electron shells. These improvements of the Stillinger–David potential allow us to reproduce successfully all essential results of quantum mechanical calculations of the interaction energy for water molecules obtained by Clementi. Analyzing the behavior of the dipole moment for water molecule as a function of inter-particle spacing, we obtain the estimate for two- and three- particle effects in water [1-4].
The generalized Stillinger–David potential is applied to the investigation of hydration problem the properties of dimer, trimer and multimer or higher order [1,3].
The physical nature of H-bond in water is discussed [5].

[1] I.V. Zhyganiuk, Ukr. J. Phys. **56**, 225 (2011).
[2] I. Zhyganiuk, Natl. Acad. Sci. Ukr **8**, 77 (2009).
[3] I. Zhyganiuk, Natl. Acad. Sci. Ukr **11**, 72 (2009).
[4] L.A. Bulavin, I.V. Zhyganiuk, N.P. Malomuzh, K.M. Pankratov, Ukr. J. Phys. **56**, 893 (2011).
[5] P.V. Makhlaichuk, N.P. Malomuzh, I.V. Zhyganiuk, Ukr. J. Phys. **57**, 113 (2012).

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