National Academy of Sciences of Ukraine Bogolyubov Institute for Theoretical Physics Young Scientists Council

VIII International Young Scientists Conference Problems of Theoretical Physics

December 12 - 14, 2017

Kyiv, Ukraine

Program & Abstracts

Kyiv 2017

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Prof. Dr. Sci. **B.I. Lev** Bogolyubov Institute for Theoretical Physics, NAS of Ukraine

Dr. Sci. **S.G. Sharapov** Bogolyubov Institute for Theoretical Physics, NAS of Ukraine

Prof. Dr. Sci. **A.G. Magner** Institute for Nuclear Research, NAS of Ukraine

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$\begin{array}{c} I \\ Program \end{array}$

VIII Young Scientists Conference Problems of Theoretical Physics

 $\begin{array}{c} {\rm December}\ 12-14,\ 2017\\ {\rm Kyiv,\ Ukraine} \end{array}$

Tuesday, December 12, 2017

| 08-30 | Registration |
|---------|-------------------------------------------------------------------------|
| 09-50 | Opening of the conference |
| | Prof. Dr. Sci. Anatoly G. Zagorodny, |
| | Academician of the NAS of Ukraine, |
| _ | Director of the Bogolyubov Institute for Theoretical Physics |
| | Morning Session |
| 10-00 | Prof. Dr. Sci. B.I. Lev |
| Lecture | "Non-equilibrium self-gravitating systems" |
| | Bogolyubov Institute for Theoretical Physics, NAS of Ukraine, Kyiv |
| 10-45 | O.I. Gerasymov, A.Ya. Spivak |
| O.1 | "Mechanical impulse transmission through 1D nonlinear chains" |
| | Odesa State Environmental University, Odesa, Ukraine |
| 11-05 | V.N. Gorev, A.I. Sokolovsky |
| O.2 | "Conservation laws for the Landau-Vlasov kinetic equation with |
| | the nonlocal collision integral" |
| | National Mining University, Dnipro |
| 11-25 | A. Vidybida, <u>O. Shchur</u> |
| O.3 | "Relation between firing statistics of spiking neuron with delayed fast |
| | inhibitory feedback and without feedback" |
| | Bogolyubov Institute for Theoretical Physics, NAS of Ukraine, Kyiv |
| 11-45 | A.G. Magner, M.I. Gorenstein, U.V. Grygoriev |
| 0.4 | "Ultrasonic waves in classical gases" |
| | Taras Shevchenko National University of Kyiv |

| 12-05 | COFFEE BREAK |
|-------|-------------------------------------------------------------------------------------|
| 12-25 | K.M. Haponenko, A.I. Sokolovsky |
| O.5 | "Nonequilibrium thermodynamic potential for Bose system in the |
| | presence of condensate" |
| | Oles Honchar Dnipropetrovsk National University, Dnipro |
| 12-45 | A.R. Kuzmak |
| O.6 | "Quantum state manifolds generated by the Lie algebra" |
| | Ivan Franko National University of Lviv |
| 13-05 | O.O. Morozko, Kh.P. Gnatenko |
| O.7 | "Many-particle system in noncommutative space with preserved |
| | rotational symmetry" |
| | Ivan Franko National University of Lviv |
| 13-25 | D.V. Piatnytskyi, S.N. Volkov |
| O.8 | "Estimation of the value of energy of broken spatial inversion |
| | symmetry at the interface between two ferromagnets" |
| | Bogolyubov Institute for Theoretical Physics, NAS of Ukraine, Kyiv |
| 13-45 | O. Zdorevskyi, S.N. Volkov |
| O.9 | "Role of water and hydrogen peroxide molecules in nucleic base pairs stabilization" |
| | Bogolyubov Institute for Theoretical Physics, NAS of Ukraine, Kyiv |
| 14-05 | LUNCH |
| | Afternoon Session |
| 15-30 | V. Sagun, Ilidio Lopes |
| O.10 | "Probing the neutron stars interior within the realistic equation of |
| | state" |
| | Bogolyubov Institute for Theoretical Physics, NAS of Ukraine, Kyiv |
| 15-50 | D. Savchenko, D. Iakubovskyi |
| O.11 | "Testing the origin of 3.55 keV line in individual galaxy clusters |
| | observed with XMM-Newton" |
| | Bogolyubov Institute for Theoretical Physics, NAS of Ukraine, Kyiv |
| 16-10 | A. Rudakovskyi, D. Iakubovskyi |
| O.12 | "Cores in fermionic dark matter haloes with maximal phase-space |
| | density" |
| | Bogolyubov Institute for Theoretical Physics, NAS of Ukraine, Kyiv |

16-30 I. Bilinsky, P. Berczik, O. Veles

O.13 "Performance testing of the TREE based modern GPU/N-body code implementation"

Main Astronomical Observatory of the National Academy of Science, Kyiv

17-30 WELCOME PARTY

Wednesday, December 13, 2017

| | Morning Session |
|---------|---------------------------------------------------------------------|
| 10-00 | Dr. S.G. Sharapov |
| Lecture | "Graphene and other Dirac materials" |
| | Bogolyubov Institute for Theoretical Physics, NAS of Ukraine, Kyiv |
| 10-45 | K.V. Germash, D.V. Fil |
| O.14 | "Non-linear electromagnetic properties of double layer graphene |
| | systems with electron-hole pairing" |
| | Institute for Single Crystals of NAS of Ukraine, Kharkiv |
| 11-05 | V.O. Shubnyi, Yu.V. Skrypnyk, S.G. Sharapov, |
| | V.M. Loktev |
| O.15 | "Effect of uniaxial strain on scattering from point defects in |
| | graphene" |
| | Taras Shevchenko National University of Kyiv |
| 11-25 | I.O. Starodub, Y. Zolotaryuk |
| O.16 | "Fluxon scattering on dipole inhomogeneity in Josephson junction" |
| | Bogolyubov Institute for Theoretical Physics, NAS of Ukraine, Kyiv |
| 11-45 | COFFEE BREAK |
| 12-05 | O.Y. Pastukh, V.E. Sakhnyuk, D.M. Shvalikovsky |
| O.17 | "The infuence of an external magnetic field on the critical current |
| | in SNINS contacts near the critical temperature" |
| | Lesya Ukrainka Eastern European National University, Lutsk |
| 12-25 | A.M. Shutowskiy, A.V. Svidzinsky, V.E. Sakhnyuk |
| O.18 | "The functional integration method in the two band |
| | superconductivity theory" |
| | Lesya Ukrainka Eastern European National University, Lutsk |
| 12-45 | V.V. Bezghuba, A.A. Kordyuk |
| O.19 | "Brillouin zone of iron-based superconductor in kz direction" |
| | Kyiv Academic University |
| 13-05 | D.Y. Kononenko, O.V. Pylypovskyi, Yu. Gaididei, |
| | D.D. Sheka |
| O.20 | "Spin waves propagation in antiferromagnetic ring" |
| | Taras Shevchenko National University of Kyiv |

| 13-25 | A.I. Korniienko, O.V. Pylypovskyi, V.P. Kravchuk, |
|-------|-------------------------------------------------------------------------|
| | D.D. Sheka, Yu. Gaididei |
| O.21 | "Magnetic metamaterials: curvature induced magnonic crystals in |
| | nanowires" |
| | Taras Shevchenko National University of Kyiv |
| 13-45 | C.M. Scherbakov, A.N. Morozovska, Yu. M. Vysochanskii |
| O.22 | "Spatially modulated incommensurate phases induced by flexoelectric |
| | coupling in ferroelectrics" |
| | Taras Shevchenko National University of Kyiv |
| 14-05 | LUNCH |
| | Afternoon Session |
| 15-15 | O. Boliasova, V. Krivoruchko |
| O.23 | "Longitudinal spin dynamics in antiferromagnets: Diagrammatic |
| 0.20 | approach" |
| | A.A. Galkin Donetsk Institute for Physics and Engineering, NAS of |
| | Ukraine, Kyiv |
| 15-35 | O.R. Sulymenko, , O.V. Prokopenko |
| O.24 | "THz-frequency AC signal source based on antiferromagnetic spin-Hall |
| | oscillator" |
| | Taras Shevchenko National University of Kyiv |
| 15-55 | L.Yu. Kharkhalis, O.O. Korolevych, O.V. Dulkai |
| O.25 | "Electronic structure of the InSe diluted magnetic semiconductors" |
| | Uzhhorod National University, Institute of Physics and Chemistry |
| | of Solid State |
| 16-15 | E.A. Eliseev, I.S. Vorotiahin, Y.M. Fomichov, M.D. Glinchuk, |
| | S.V. Kalinin, Y.A. Genenko, A.N. Morozovska |
| O.26 | "Flexo-chemical coupling in ferroelectric thin films with defect layer" |
| | Institute for Problems of Materials Science, NAS of Ukraine, Kyiv |
| | Charles University, Prague, Czech Republic |
| 16-35 | S.E. Reschikoff |
| O.27 | "The bias error of flicker noise spectral exponent estimation" |
| | Ulyanovsk State Technical University, Ulyanovsk , Russia |
| 16-55 | O.A. Hrebnov, V.F. Korolovych, L.A. Bulavin, L.Yu. Matsuy |
| O.28 | "Dielectric properties of nanocellulose aqueous suspension" |
| | Taras Shevchenko National University of Kyiv |
| 16-55 | A.V. Bezvershenko, A.K. Kolezhuk, B.I. Ivanov |
| O.29 | "Stabilization of magnetic skyrmions by RKKY interactions" |
| | Taras Shevchenko National University of Kyiv |

Thursday, December 14, 2017

| | Morning Session |
|---------|-----------------------------------------------------------------------|
| 10-00 | Dr. A.G. Magner |
| Lecture | "Kinetic approaches to the collective nuclear-matter dynamics" |
| | Institute for Nuclear Research, NAS of Ukraine, Kyiv |
| 10-45 | O. Ivanytskyi, K. Bugaev, E Nikonov, E-M. Ilgenfritz, |
| | V. Sagun, I. Mishustin, V. Petrov, G. Zinovjev |
| O.30 | "The liquid droplet view on the phase transition in $SU(2)$ |
| | gluodynamics" |
| | Bogolyubov Institute for Theoretical Physics, NAS of Ukraine, Kyiv |
| 11-05 | R.V. Poberezhnyuk |
| O.31 | "Quantum van der Waals model versus Walecka model of nuclear |
| | matter" |
| | Bogolyubov Institute for Theoretical Physics, NAS of Ukraine, Kyiv |
| 11-25 | N.V. Kolomoyets, V. Skalozub |
| O.32 | "Color structure of magnetic mass of chromomagnetic field" |
| | Oles Honchar Dnipropetrovsk National University, Dnipro |
| 11-45 | P. Minaev, V. Skalozub |
| O.33 | "Electroweak phase transition in a spontaneously magnetized vacuum" |
| | Oles Honchar Dnipropetrovsk National University, Dnipro |
| 12-05 | O. Panova |
| O.34 | "Cumulative production of nucleons by heavy baryonic resonances in |
| | proton-nucleus collisions" |
| | Taras Shevchenko National University of Kyiv |
| 12-25 | A. Pevzner, V. Skalozub |
| O.35 | "Possibility of the Abelian Z' with a non-narrow resonance within the |
| | model-independent approach" |
| | Oles Honchar Dnipropetrovsk National University, Dnipro |
| 17-35 | Juri consultation |
| 17-50 | Closing of the conference |

Statistical Theory of Many-Body Systems

Mechanical impulse transmission through 1D nonlinear chains

O.I. Gerasymov, A.Ya. Spivak

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In this work, we perform a specific class of equations, which governs mechanical impulse transportation through 1D nonhomogeneous chain with nonlinear interactions. Basic equation, which describe impulse transition, traditionally can be written in following discrete form [1]:

$$m\frac{\partial^2 z_n}{\partial t^2} = C\varepsilon_{n-1}^{\delta} - C\varepsilon_n^{\delta} + F(0)_n, \tag{1}$$

where z_n - is a position of n-th particles in chain of identical masses m; $\varepsilon_n = a - (z_{n+1} - z_n)$ - is a overlap between (n+1)-th and n-th particles, which depend from contact force $F = C\varepsilon^{\delta}$; C - is a force constant, which depend from constitutive property, size and form of particles; a - is a particle diameter; δ - is a nonlinear parameter, which for spheres is 3/2; $F_n(0)$ - is a initial force. Taking the continous limit of Eq.(1) we obtain a specific class of nonlinear partial differential equations which are able to describe the dynamics of excitations with a controlled accuracy. Namely:

$$\frac{1}{\gamma} \cdot \frac{\partial^2 \varepsilon}{\partial t^2} = a^2 \frac{\partial^2}{\partial t^2} \left(\varepsilon^{\delta} \right) + \frac{a^4}{12} \cdot \frac{\partial^2}{\partial t^2} \left(\varepsilon^{\delta} \right). \tag{2}$$

In particular when F(0) = 0 and $\delta = 3/2$, we found Eq.(2) satisfied by the following solution $\varepsilon = \varepsilon_{max} \cdot \cos^4 \frac{h-vt}{\sqrt{3}a}$ (where $\varepsilon_{max} = \frac{36v^4}{25a^4\gamma^2}$ - is a maximum of particles overlap; v - is a soliton velocity; $\gamma = C/m$ - is a new force constant), which is known as Nesterenko's soliton mode [2-4] (with some deviations in amplitudes and velocities).

We conclude the mechanical excitations of low-dimensional nonlinear chain with nonhomogenities could be transmitted as a nonlinear mode (soliton-like) if initial dispersion is not larger then Nesterenko's soliton dispersion. In the opposite case we have a dispersive wave mode with decay of amplitudes.

- [1] O.I. Gerasymov, N. Vandewalle, Dopov. Nac. acad. nauk Ukr. Rep. Nat. Acad. Sc. Ukr. no.8, 67 (2012). (in Ukrainian)
- [2] V.F. Nesterenko, J. Appl. Mech. Tech. Phys. **24**, 733 (1984).
- [3] C. Coste, E. Falcon, S. Fauve, Phys. Rev. E **56**, 6104 (1997).
- [4] C. Daraio, V.F. Nesterenko, E.B. Herbold, S. Jin, Phys. Rev. E **73**, 026610 (2006).

Conservation laws for the Landau–Vlasov kinetic equation with the nonlocal collision integral

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We consider a one-component weakly non-uniform gas with small potential interaction. The basis of investigation is the kinetic equation up to the second order in small interaction with the general nonlocal collision integral. This kinetic equation can be obtained on the basis of the Bogolyubov reduced description method [1] and in case of local collision integral it gives the known Landau–Vlasov kinetic equation.

Usually the hydrodynamics is built on the basis of the kinetic equation with the local collision integral, but, as known, the Burnett (i.e. the second-order is small gradients) approximation meets some difficulties. Maybe, in some cases these difficulties can be overcome by taking into account the nonlocality of the collision integral. So, it is an interesting problem to investigate the system hydrodynamics on the basis of the nonlocal collision integral.

The hydrodynamic reduced description parameters (RDPs) are usually chosen as the densities of the conserved quantities, i.e. the particle number, the momentum and the kinetic energy densities. Here it is shown that although the kinetic energy of the system is conserved on the basis of the local collision integral, it is not conserved on the basis of the nonlocal collision integral. So, the use of the kinetic energy as a RDP is unreasonable even for a model problem with an omitted Vlasov term. It is shown that the system total energy which is the sum of the kinetic and potential energies is conserved up to the second order both in small interaction and in small gradients. So, the following set of RDPs should be chosen: the particle number density, the momentum density and the total energy density.

The fluxes of the RDPs are calculated in terms of the one-particle distribution function in the leading-in-gradients order. It is also shown that the momentum and total energy flux densities do not contain the linear-in-gradients terms in the first order in small interaction. This fact justifies our results, because, as is known, the Vlasov term is not important for the calculation of the system kinetic coefficients.

The obtained results can be applied to the calculation of the fluxes in the first order in gradients and for the construction of the hydrodynamics on the basis of the nonlocal collision integral with the help of the Chapman–Enskog method.

[1] A.I. Akhiezer and S.V. Peletminsky, Methods of Statistical Physics, Oxford, Pergamon Press, 1981, 376 p.

Relation between firing statistics of spiking neuron with delayed fast inhibitory feedback and without feedback

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We consider a class of spiking neuronal models, defined by a set of conditions typical for basic threshold-type models, such as the leaky integrate-and-fire or the binding neuron model and also for some artificial neurons. A neuron is fed with a renewal process. Each output impulse is applied to the neuron itself after a finite delay Δ . This impulse acts as being delivered through a fast *Cl*-type inhibitory synapse. We derive a general relation which allows calculating exactly the probability density function (pdf) p(t) of output interspike intervals of a neuron with feedback based on known pdf $p^0(t)$ for the same neuron without feedback, and on the properties of the feedback line (the Δ value). Similar relations between corresponding moments are derived.

Furthermore, we prove that initial segment of pdf $p^0(t)$ for a neuron with a fixed threshold level is the same for any neuron satisfying imposed conditions, and is completely determined by the input stream. For the Poisson input stream, we calculate that initial segment exactly and, based on it, obtain exactly the initial segment of pdf p(t) for a neuron with feedback. That is the initial segment of p(t) is model-independent as well. The obtained expressions are checked by means of Monte Carlo simulation. The course of p(t) has a pronounced peculiarity, which makes it impossible to approximate p(t) by Poisson or other simple stochastic process.

Ultrasonic waves in classical gases

A.G. Magner¹, M.I. Gorenstein², U.V. Grygoriev³

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The velocity c_r and absorption coefficient γ for plane sound waves in a classical gas are obtained by solving the Boltzmann kinetic equation with a collision term in the τ -relaxation time approximation. This equation describes a reaction of the single-particle distribution function $f(\mathbf{r}, \mathbf{p}, t)$ in the phase-space coordinates \mathbf{r} and momentum \mathbf{p} , and time t to a periodic external field oscillating with a frequency ω ($c = \omega/(v_T k_r) = c_r + i c_i$, $v_T = (2T/m)^{1/2}$, T is the system temperature and m the particle mass, $k = k_r + i k_i$). Within the linear response theory (LRT), the non-perturbative dispersion equation valid for all of sound frequencies ω is derived and solved numerically. Figure shows the results that are in agreement with the frequent (FCR, $\omega \tau \ll 1$) and rare (RCR, $\omega \tau \gg 1$) collision-regime approximations. These results are also in qualitative agreement with the experimental data for ultrasonic waves in dilute gases. The thermal conductivity will be calculated in future work.

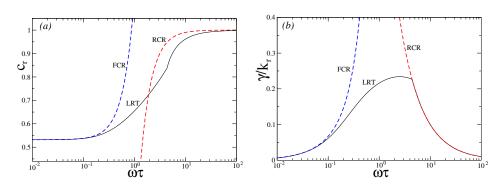


Figure 1 The scaled velocity c_r in the v_T units (a) and absorption coefficient γ/k_r (b) as functions of the Knudsen parameter $\omega\tau$. Solid lines show the nonperturbative LRT solutions. Dashed lines present the asymptotic FCR and RCR approximations.

[1] A.G. Magner, M.I. Gorenstein, and U.V. Grygoriev, Phys. Rev. E **95**, 0521113 (2017); arXiv:1710.03630 v1 [cond-mat.stat-mech] 2017.

Nonequilibrium thermodynamic potential for Bose system in the presence of condensate

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Bose system in the presence of condensate is investigated in the Bogolyubov model of the separated condensate (see about in [1]). In this state occupation number n_0 of one-particle state with momentum $\vec{p} = 0$ is macroscopic one. In this model the system is described by the statistical operator

$$w(n_0) = e^{\beta \left[\Omega(n_0) - \hat{H}(n_0) + \mu \hat{N}(n_0)\right]}$$
 Sp $w(n_0) = 1$

where operators $\hat{H}(n_0)$, $\hat{H}(n_0)$ are given by Hamiltonian of the system \hat{H} and operator of particle number \hat{N} after substitution $n_0^{1/2}$ instead of the Bose operators a_0, a_0^+ (β , μ are the reverse temperature and the chemical potential). According to Bogolyubov equilibrium value n_0^o of the occupation number n_0 can be found from the minimum condition of the thermodynamic potential $\Omega(n_0)$ i.e. it is the nonequilibrium one of the system. Near transition point from normal state to the state with the condensate occupation number n_0 is small and the potential $\Omega(n_0)$ can be calculated in a perturbation theory in powers of $n_0^{1/2}$.

The purpose of this paper is calculating of the potential $\Omega(n_0)$ in a modified thermodynamic perturbation theory with small parameter n_0 . The obtained expression for $\Omega(n_0)$ can be used as the potential Landau in his theory of the phase transitions of the second kind for the system under consideration. The calculation is conducted up to the sixth order terms of the perturbation theory in powers of the occupation number n_0 inclusive. It is shown that only integer powers of this number are present in the corresponding series and the potential has the structure $\Omega(n_0) = \Omega(0) + \sum_{s=0}^{6} a_s(\beta, \mu) n_0^s + O(n_0^7)$. Relatively compact expressions for the coefficients $a_s(\beta, \mu)$ are obtained because operators describing the interaction in the system commutate under T-product. For a Bose gas they are calculated in an additional perturbation theory in interaction between particles. Detailed analyze of the results with connection to the Landau theory of phase transitions will be given in another paper.

1.A.I. Akhiezer and S.V. Peletminskii, Methods of Statistical Physics, Oxford, New York:Pergamon Press, 1981, 450 p.

Mathematical Physics

Quantum state manifolds generated by the Lie algebra

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We study the Fubini-Study metrics of quantum state manifolds generated by the Heisenberg and so(3) Lie algebras. Using these results the metrics of state manifolds generated by the position and momentum operators are calculated. Also the metrics of quantum state manifolds generated by some spin systems are obtained. Finally, we generalize this problem for an arbitrary Lie algebra.

Many-particle system in noncommutative space with preserved rotational symmetry

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In noncommutative space operators of coordinates and operators of momenta satisfy the following commutation relations

$$[X_i, X_j] = i\hbar\theta_{ij},\tag{3}$$

$$[X_i, P_i] = i\hbar \delta_{ij},\tag{4}$$

$$[P_i, P_j] = 0. (5)$$

In the canonical version of noncommutative space θ_{ij} are elements of constant anti-symmetric matrix.

We consider noncommutative space which is equivalent to noncommutative space of canonical type (1)-(3) and is rotationally-invariant [1,2]. The noncommutative space is proposed on the basis of idea of generalization parameters of noncommutativity θ_{ij} to tensors. The tensors are constructed with the help of additional coordinates which are governed by rotationally-symmetric system.

In the general case different particles may feel noncommutativity with different tensors. Therefore there is a problem of describing the motion of the center-of-mass of a system in rotationally-invariant noncommutative space. We analyze commutation relations for coordinates of the center-of-mass of composite system, for coordinates of the relative motion. We conclude that the coordinates of the center-of-mass satisfy noncommutative algebra with effective tensors of noncommutativity. We also find that coordinates of the center-of-mass and coordinates of the relative motion do not commute. Therefore the motion of the center-of-mass and the relative motion are not independent in rotationally-invariant noncommutative space.

We find condition on which the effective tensors of noncommutativity that describe the motion of the center-of-mass of composite system depend on its total mass and do not depend on its composition. Moreover, in the case when the condition is satisfied the coordinates of the center-of-mass and coordinates of the relative motion commute, therefore the motion of the center-of-mass and the relative motion are independent.

- [1] Kh. P. Gnatenko, V. M. Tkachuk, Phys. Lett. A 378, 3509 (2014)
- [2] Kh. P. Gnatenko, V. M. Tkachuk, Ukr. J. Phys. **61**, 432 (2016) .

Physics of Biological Macromolecules

Complexes of hydrogen peroxide and DNA phosphate group

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The effect of DNA destruction or deactivation during particle irradiation of living cells is widely used in cancer therapy. Despite the wide development of the methods of ion therapy for treating cancer the mechanism of DNA damage is still being discussed [1]. There are some theories, which include damage by secondary electrons, oxidative stress by OH-radicals, shock-wave damage etc. It was proposed in [2] that DNA deactivation can be a result of intracellular medium change after irradiation. The emphasis was made on molecules of hydrogen peroxide (H_2O_2) formed in the radiolysis process during the irradiation of water medium. It is shown in Monte-Carlo simulations, that H_2O_2 molecule is one of the most long-living products of water radiolysis [3]. Peroxide molecule can diffuse on considerable distances in the cell after irradiation and reach the active sites of DNA macromolecule.

The question is how hydrogen peroxide can interact with DNA. The most appropriate and convenient place of interaction can be phosphate groups, because they are situated on the DNA backbone and carry negative charge. In the present work the geometry optimizations and calculations of energies are carried out for complexes, which consist of hydrogen peroxide molecule, water molecule, phosphate group and sodium counterion using Hartree-Fock, MP2 and density functional theory methods in Gaussian 03 software.

It is shown, that molecule of hydrogen peroxide can form the relatively stable complex with phosphate group and sodium counterion similarly to water molecule. But, H_2O_2 molecule can remain near DNA strand longer than H_2O molecule, because H_2O_2 is nearly twice as heavy as water molecule, and thus, blocks genetic activity of DNA. Also, being in complex with PO_4 groups, the hydrogen peroxide molecules can decay into OH-radicals in close proximity to DNA backbone and induce double strand breaks.

- [1] M. Krämer, M. Durante, Eur. Phys. J. D **60**, 195 (2010).
- [2] D.V. Piatnytskyi, O.O. Zdorevskyi, S.M. Perepelytsya, S.N. Volkov, Eur. Phys. J. D **69**, 255 (2015).
- [3] M.S. Kreipl, W. Friedland, H.G. Paretzke, Radiat. Environ. Biophys. 48, 11 (2009).

Role of water and hydrogen peroxide molecules in nucleic base pairs stabilization

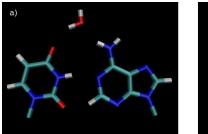
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Water environment is an important factor in DNA secondary structure stabilization. It was shown [1] that during genetic information transfer process under certain conditions base pairs can transit into some 'pre-opened' metastable state. It is known [2] that on the stabilization of this state significantly influences interaction with molecules from the surrounding medium.

In the present work DNA nucleic base pairs stability is investigated in the presence of water and hydrogen peroxide molecules. Interaction energies are calculated using atom-atom potential functions method. Van der Waals, Coulomb interactions and hydrogen bonds are taken into account.

As a result it was shown that hydrogen peroxide molecules can create stable long-living complexes with DNA base pairs compared to the same complex with water molecule (Fig. 1). As hydrogen peroxide is highly accumulated in the medium during ion beam cancer treatment [3] this can be a key factor in the termination of cancer cells duplication in the process of ion therapy.



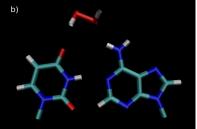


Figure 2 Complexes of adenine-thymine DNA base pair with: a) water molecule; b) hydrogen peroxide molecule.

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Astrophysics and Cosmology

Probing the neutron stars interior within the realistic equation of state

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A novel equation of state with the surface tension induced by particles' interaction was generalized to describe properties of the neutron stars [1, 2]. In such equation the interaction between particles is done via the hard-core repulsion by taking into account the proper volumes of particles. Recently, this model was successfully applied to the description of the properties of nuclear and hadron matter created in collisions of nucleons. The new approach is free of causality problems and fully thermodynamically consistent which enables us to use it to the investigation of the strongly interacting matter phase diagram properties in wide range of temperatures and baryon densities, including neutron stars. Here, we calculated the mass-radius relations for a compact star using the Tolmann-Oppenheimer-Volkov equation for two sets of parameters which satisfy the existing constraints. Accordingly, we found the parameter values that are in good agreement with the same ones obtained from the nuclear-nuclear collision data analysis [2]. The astrophysical constraints suggest that the hard-core radius of baryons can vary between 0.476 fm and 0.5 fm.

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Testing the origin of ~ 3.55 keV line in individual galaxy clusters observed with XMM-Newton

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If the unidentified emission line at ~ 3.55 keV previously found in spectra of nearby galaxies and galaxy clusters is due to radiatively decaying dark matter, one should detect the signal of comparable strength from many cosmic objects. We selected 20 galaxy clusters with the largest dark matter column densities within the 14' radius circle roughly corresponding to Field-of-View of XMM-Newton X-ray cosmic mission. Omitting Abell 539 that was not observed by XMM-Newton, we analyzed the XMM-Newton/EPIC observations of the remaining sample of 19 clusters. In 5 of them, we identified 2σ positive line-like residuals with average position 3.56 ± 0.02 keV in the emitter's frame. Their observed properties are unlikely to be explained by statistical fluctuations (having roughly 3σ significance of line signal). They can't be explained by astrophysical emission lines because known atomic lines are included in the fitting model. The redshift dependence of the best-fit line energies makes an additional argument against general-type systematics.

Cores in fermionic dark matter haloes with maximal phase-space density

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We formulate a new model of dark matter distribution for any type of dark matter fermions (Iakubovskyi & Rudakovskyi, in prep.). Our model has only one extra parameter – the maximal value f_{max} of dark matter phase-space density – that turns a cusped Navarro-Frenk-White density profile into a cored one. Despite its simplicity, our model successfully reproduces cored dark matter profiles from N-body simulations with warm dark matter (having finite f_{max}). Also, we have obtained the scaling relation between f_{max} (or, equivalently, the mass of dark matter fermions) and the dark matter core radius in dSphs. Finally, we estimated the influence of velocity anisotropy on the cored density profile by using the Osipkov-Merritt model and calculated the density profiles of the typical dSphs for different masses of fermionic dark matter particle and different anisotropy parameters r_a . It was obtained that the influence of velocity anisotropy on the cored density profile is small for all physically motivated values of r_a .

Performance testing of the TREE based modern GPU/N-body code implementation

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We develop a new version of the N-body TREE-GRAPE (GRAvity PipEline) code (Fukushige et al. 2005, Section 4.1). We ported the original GRAPE-based tree code to many different hardware platforms, including the CPU (with multithread usage under the SSE or AVX instructions) and also to the recent NVIDIA Graphics Processing Unit (GPU) platform using the Compute Unified Device Architecture (CUDA). In order to efficiently use the current acceleration hardware (GPU), we employed a modified tree algorithm, originally developed by Barnes & Hut (1986), which was first used on GRAPE-1 A by Makino (1991) and Fukushige et al. (1991).

On a typical desktop hardware (CPU: i5-2500K with 4 cores at 3.3 GHz + GPU: GeForce GTX 570 with 480 cores at 1.46 GHz) we get the results for the full self-gravity force calculation routine with the typical tree-construction para-meters (θ = 0.5, ng = 3500, (Fukushige et al. 2005, Section 4.1.1)) for N = 1M particles with the initial Plummer distribution in ~2 sec. Our speed is quite comparable to the most advanced and recent fully GPU tree-code implementation (bonsai2: Bédorf et al. 2012), which does one full force calculation on the same hardware for the same particle distribution and with the same opening angle in ~1 sec. In the future we plan to use our hardware-accelerator-based gravity calculation routine in a few new galactic dynamics projects which include also the Supermassive Black Hole merger dynamics and Gravitational Wave emissions from such a sources.

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Condensed Matter Physics

Non-linear electromagnetic properties of double layer graphene systems with electron-hole pairing

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The double layer graphene systems are considered as promising candidates for realizing the electron-hole pairing [1]. The systems consist of two conducting graphene sheets, in which the one sheet has an electron-type conductivity, and the other has a hole-type conductivity. At low temperature electrons and holes from the opposite layers form pairs similar to Cooper pairs in superconductors. It is important to find the effects that are a hallmarks of the electron-hole pairing. Recently it was shown that the electron-hole pairing reduces significantly screening properties [2], modifies the spectrum of plasmons [3], and causes the strong resonant absorption and reflection of electromagnetic waves [3] in double layer graphene systems.

In this report we study the influence of the electron-hole pairing on non-linear (NL) electromagnetic properties of double layer graphene systems. The double mono-layer and double bilayer graphene systems are considered. The density matrix approach [4] is used to calculate the NL response to the external electromagnetic field. The NL conductivities of the second and third order are found.

The effect of strong enhancement of third-harmonic generation (THG) is predicted [5]. The effect manifests itself in the appearance of the peaks in the THG intensity. The peaks correspond to the incident photon energies $\hbar\omega$ equal to $(2/3)\Delta$, Δ , $(2/3)\sqrt{\epsilon_F^2 + \Delta^2}$, where ϵ_F is the Fermi energy and Δ is the order parameter of the electron-hole pairing.

The NL mechanism of plasmon generation that use difference frequency wave mixing is investigated. Intensities of generation of surface plasmons caused by second-order and third-order nonlinearities in double layer graphene systems are evaluated.

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Effect of uniaxial strain on scattering from point defects in graphene V.O. Shubnyi¹, Yu.V. Skrypnyk², S.G. Sharapov², V.M. Loktev^{2,3}

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Recent experimental study of the far-infrared transmission spectra of large area chemical-vapor-deposited monolayer graphene [1] has shown that the Drude peak width increases by more than 10% per 1% of applied uniaxial strain, while the Drude weight and the Fermi energy remain unchanged. Whereas in the original experimental work the strong effect is attributed to the surface phonons, we propose an alternative explanation based on the inevitable presence of some amount of impurities in the experimental samples.

In metals impurities can contribute to the increase in the Drude peak width due to reduced inter-site hopping integrals in the strained sample. However, in the commonly considered case of weakly scattering impurities, this effect is quite moderate for any reasonable impurity concentration. On the contrary, we argue that resonance impurities, which are characterized by strong scattering potentials, may account for the observed magnitude of the effect. It is shown that the existence of a well-defined single impurity resonance is the necessary condition for the enhancement of the peak widening under a strain. Such an enhancement arises from the gradual shift of the impurity resonance energy, which results from the impurity interaction with the host crystal, towards the Dirac point with increasing the strain. Thus, when the Fermi level is positioned closer to the Dirac point than the resonance energy, it finds itself in the domain of the significantly increased impurity scattering with applying the strain. The enhancement of the peak widening is the most prominent when the Fermi energy is located near the half height of the resonance.

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Fluxon scattering on dipole inhomogeneity in Josephson junction

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The dynamics of fluxon or magnetic flux quantum in the dielectric layer of Josephson junction with presence of time-independent bias, dissipation and spatial inhomogeneity is examined. Fluxons are represented as a solitary waves which are the solutions of the sine-Gordon equation on the difference of the wave function phase of the superconducting condensate [1]. The qubit existence in Josephson junction can be presented as the spatial dimensional inhomogeneity with different polarity on the way of fluxon motion [2]. The fluxon scattering on the dipole inhomogeneity of the step-function form is investigated. The equations of fluxon motion in Josephson junction with dipole inhomogeneity which models the qubit are found. The dynamics of fluxon has a great dependence from inhomogeneity size parameters. The threshold current which is the minimum current needed for fluxon to pass an obstacle is found analytically with help of modified balance equation method [3]. This current depend on impurity size and dissipation in the junction. Numerical results show a great dependence of threshold current to impurity length, particularly, that there is some "optimal" value of it exists after reaching of which the length of impurity does not influence on the threshold current. When the fluxon interacts with impurities in two different states its velocity changes differently too, thus, the delay time between such fluxons in the observation point is appearing. The numerical simulations of fluxon dynamics with respect of Runge-Kutta method were performed. The obtained results show the delay time decreasing while velocity increasing and almost tend to zero on relativistic velocities. The delay time is greater when inhomogeneity size is larger. The analyze of delay time gives an opportunity to read out the state of impurity, hence, the state of the qubit.

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The influence of an external magnetic field on the critical current in SNINS contacts near the critical temperature

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The behavior of the superconducting contact of SNINS-type (where S - superconductor, N - normal metal, I - insulator) in the external magnetic field is investigated. The behavior of the Josephson contacts in a magnetic field is well studied for the case of the traditional sinusoidal current-phase relation [1]. The dependence of the maximum current on the magnitude of the magnetic flux was investigated for superconducting SIS junction for a wide range of electron transmission coefficients in [2].

In this research was found out, how the presence of a normal layer of arbitrary thickness and dielectric film with a wide range of changes of electron transmission coefficient affects on the sensitivity of maximum current to the magnitude of the magnetic field in SNINS contact. In addition, the influence of non-magnetic impurities of arbitrary concentration in such a contact was analyzed. As it was found out, with the increase of the electron transmission coefficient, the critical current in the contact becomes much more sensitive to the change of magnetic flux, which is especially noticeable when the magnetic flux values are close to the integer number of the elemental flow quantum. Also was shown that increase of the concentration of nonmagnetic impurities leads to a decrease in the magnitude of the current maximum.

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The functional integration method in the two band superconductivity theory

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The Poisson parametrization [1] helps to obtain the partition function representation of a one band superconductor in the functional integral form. This approach works in the two band superconductivity theory [2] too.

The interaction representation [3] introduces the ordered exponential concept. Considering the ordered exponential as a product of exponentials we have obtained the representation of the Bloch equation solution in the functional integral form in the two band superconductivity case. The graduation from evolution operator to partition function of a two band superconductor is known. It gives a possibility to calculate the thermodynamic potential approximately. Using the obtained partition function representation we have formulated a mean field approximation tested in the functional integral theory. We have introduced two complex functions called order parameters. These functions characterize a superconducting state of a two band superconductor.

Using the bilinear Hamiltonian we have obtained a possibility to construct the current density expression of different superconducting tunnel junctions based on two band superconductors. Every quantity has been defined in terms of Matsubara Green functions.

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Brillouin zone of iron-based superconductor in k_z direction

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Nowadays the nature of high-temperature superconductivity (HTSC) remains unclear. There are many different theoretical models, which describe some of HTSC aspects and peculiarities, but none of them is neither fully predictive nor coherent enough. Because of the extremely complicated electronic structure, the iron-based superconductors (IBS) are one of the most interesting classes of HTSC to study. In particular, the effect of three-dimensionality of electronic structure on electronic properties of IBS is not clear at all.

Using angle-resolved photoemission spectroscopy (ARPES) we have measured and studied the kz-dependence of electronic structure in BKFA, the most studied IBS. We focus on peak positions of unoccupied bands in different points of Brillouin zone, Fermi surface and renormalization dependencies. A number of unexpected effects have been observed:

- comparison of experimental results and band structure calculations hints to the swap of known excitation energy values for Γ and Z points in BKFA;
- it is identified for the first time that in addition to the band structure, renormalization in BKFA has kz-dependence as well.

Spin waves propagation in antiferromagnetic ring

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Astonishing headway in nanotechnology brings forth a great interest to nanosized magnetic objects of curved geometry because of their unique properties and crucial application potential [1]. Recent theoretical studies of curved magnetic nanosystems (e.g. low-dimensional magnets, thin shells) introduce a general approach of geometry-induced effects description [2]. For instance, magnetochiral effects in wires and ribbons were explained [3]. To the date most studies of curved nanomagnets have been focused on ferromagnetic materials.

Henceforth, in this study we propose an expansion of developed in [2] approach for curved antiferromagnets description.

In our study we consider an antiferromagnet in the frame of sigma-model approach [4] where its statics and dynamics are described in terms of Néel vector only. This description is valid for low-frequency and long-wave spectral regions.

We illustrate the developed approach by thin ring-shaped two-sublattice antiferromagnet with hard axis anisotropy oriented along the wire. We show that a normal to the ring plane distribution of Néel vector provides a global energy minimum of the system. Likewise, linear excitations of the ground state are four-times degenerated.

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Magnetic metamaterials: curvature induced magnonic crystals in nanowires

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Metamaterials, artificial periodic structures with promising advantages for control of wave propagation, are of great importance for modern nanotechnology. Metamaterials for optics (photonic crystals) are used for manipulation electromagnetic waves at optical frequencies at the nanometer scale. Nowadays, the concept of nanopatterned structure is encapsulated in different fields of physics, like as physics of phonons or plasmons. In magnetism magnonic crystals construct media for the control of magnons propagation. Magnonic crystals are the artificial magnetic structures with periodic distribution of the constituent materials or periodic modulation of magnetic parameters [1]. They are promising for all-magnon data processing [2] and used for the realization of logic operations [3].

In current study we propose the concept of curvature induced magnonic crystals with periodic spatio-inhomogeneous curvature distribution. We consider a planar ferromagnetic meander-like nanowire with strong easy-tangential anisotropy, composed of periodically arranged semi-circle segments. We describe statics and dynamics of the magnetization using the recently developed approach [4] for arbitrary shaped wires. The curvature of the system leads to appearance of geometrically induced Dzyaloshinskii-Moriya interaction and an additional anisotropy in plane of the sample, which results in a deviation of the magnetization from the strictly tangential distribution. The ground state magnetization distribution is derived analytically for the curved wire with the periodic spatial dependent curvature.

Ground state of the magnetization has periodic structure and plays a role of periodic potential for magnon excitations. The spin-wave spectrum of this structure is calculated analytically in the empty lattice approximation, which corresponds to the weak curvature case. Bandgaps in magnon spectrum are determined by the curvature. The minimal size of the gap corresponds to zero wave-vector and it decreases with the curvature amplitude increasing. There is a critical value of the curvature when the gap vanishes.

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Spatially modulated incommensurate phases induced by flexoelectric coupling in ferroelectrics

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Within Landau-Ginzburg-Devonshire (LGD) theory framework [1]-[4], analytical solutions for the soft transverse acoustic (TA) and optic (TO) phonon dispersion relations depended on the magnitude of the flexoelectric coefficient f and temperature T in linearized form where found exactly. Existence of the incommensurate modulations of wave frequency in a temperature range lower than Curie temperature T_C but higher than the temperature of incommensurate phase transition T_{IC} , $T_{IC} < T < T_C$ and under condition of the flexocoefficient magnitude ranging over the critical value, $|f| > f^{cr}(T)$, was established. We predicted the appearance of the "rippled" flexocoupling-induced incommensurate phase in the initially commensurate ferroics. Impact of the dynamic flexocoefficient M, suggested in [5], on phonon spectra was studied. It was shown that in the vincinity of a critical value of the dynamic flexocoefficient $M^{cr} = \sqrt{\mu \cdot \rho}$, where ρ is the density of a ferroic and μ is kinetic coefficient, dispersion relation has singularity. It can put to the test magnitude of the dynamic flexocoefficient in sense of the question of existence of dynamic flexoelectric coupling.

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Longitudinal spin dynamics in antiferromagnets: Diagrammatic approach

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Lately the properties of magnetic materials have been studied intensively. Nonetheless the mechanism underlying femtosecond laser-pulse-induced ultrafast magnetization dynamics remains elusive. Microscopic theoretical consideration of spin dynamics can shed light on this phenomenon. However, the longitudinal spin dynamics is less investigated than the transverse one. In particular, the longitudinal spin dynamics in an antiferromagnet is not completely understood even in equilibrium state.

In our research, the diagrammatic technique for spin operators was used to studying the longitudinal dynamics in antiferromagnets. Our consideration is based on the Heisenberg model of an antiferromagnet. The diagrammatic technique for spin operators is exact from the quantum mechanics point of view than other methods. In this case, the equations that describes the behavior of the system can be represented graphically. So, we are working with graphic objects. The graphical elements are the Green functions and the interaction integrals. Due to certain rules, the graphical representation can be replaced by equations again.

Strong renormalization of the magnetization longitudinal vibration due to a few channels of virtual creation and annihilation of transverse spin waves has been found. Videlicet, there is a process of creation and annihilation of two spin waves at frequencies $\omega(q) = \varepsilon_k - \varepsilon_{k\pm q}$ which corresponds to in-phase sublattice magnetization precession and is in close analogy to a ferromagnet [1] and ferrimagnet [2] cases. The second channel is a two-spin-wave creation/annihilation process at frequency $\omega(q) = \varepsilon_k + \varepsilon_{k\pm q}$. (In all these processes the wave vector k is a variable.) The first channel is controlled by the occupation factor determined through the spin wave Bose distribution function. However, the processes of creation or annihilation of two a two spin waves remain effective even in the absence of thermal excitations, i.e., when $n(\varepsilon_k) \to 0$, and, in our opinion, most likely provide the main contribution to the thermally induced magnetization reversal.

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THz-frequency AC signal source based on antiferromagnetic spin-Hall oscillator

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We propose a novel approach for the creation of THz-frequency AC signal source based on antiferromagnetic spin-Hall oscillator (SHO) – a layered structure consisting of a current-driven normal metal (NM) with strong spin-orbit interaction and a layer of a canted antiferromagnet (AFM). The use of AFM provides a substantial increase of the SHO operational frequencies (up to 10 THz) in comparison to the traditional ferromagnetic spin-torque oscillators [1, 2].

In the considered SHO the magnetization vectors of the AFM sublattices are canted inside the easy plane by the Dzyaloshinskii-Moriya interaction (DMI) resulting in the appearance of the small net magnetization vector \mathbf{m}_{DMI} . When a DC electric current is flowing in the NM layer, it creates, due to the spin-Hall effect, a perpendicular spin current that excites the uniform rotation of the \mathbf{m}_{DMI} . This rotating magnetization can be considered as a system of two almost identical orthogonal oscillating dipoles creating a dipolar AC field, which can be registered by an appropriate electrodynamic system.

We demonstrate theoretically that the dipolar AC power received from such AFM-based SHO can be calculated as:

$$P_{\rm AC} = P_{\rm m} \frac{V}{V_{\rm eff}} Q ,$$

where $P_{\rm m}=\mu_0 m_{\rm DMI}^2 Vf$ is the characteristic AC power generated by the rotating magnetization $\mathbf{m}_{\rm DMI}$, μ_0 is the vacuum permeability, f is the frequency of the generated AC signal, V is the volume of the AFM layer, $V_{\rm eff}$ is the effective frequency-dependent volume of a particular THz-frequency system coupled to the SHO and Q is the frequency-dependent quality factor of this system. Our calculations show that such sources can have AC power $P_{\rm AC}>1\mu{\rm W}$ and, therefore, could be suitable many practical applications. The publication contains results of the studies conducted under the "President's of Ukraine" grant for competitive projects (F74/150–2017) and grant F76/63–2017 of the State Fund for Fundamental Research of Ukraine, grants 16BF052–01 from KNU and 7F from NASU.

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Electronic structure of the InSe diluted magnetic semiconductors L.Yu. Kharkhalis, O.O. Korolevych, O.V. Dulkai

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Owing to the layered crystal structure and anisotropic physical properties binary semiconductors of indium selenides of the $A^{III}B^{VI}$ type are very interesting and perspective materials for spintronic investigations. The existence of the van der Waals coupling between the structural units allows easily to intercalate the InSe crystal by various magnetic impurities and thus influence on its magnetic properties. The authors of experimental researches [1,2] showed that InSe crystals intercalated with transition metal impurities with an unclosed d-shells (Mn, Fe, Co, Ni) exhibit the ferromagnetic order. According to data [1,2], the introduction of impurity atoms by means of intercalation in a magnetic field leads to hysteresis loops which is typical for the ferromagnetics. The values of the Curie temperature and the coercive force [2] are also obtained for the considered materials.

In this report, using first-principles pseudopotential method within density-functional theory the electronic and magnetic properties of the InSe layered crystal in the different modifications doped with 3d- elements have been investigated. We studied the possible ways intercalation of magnetic 3d -elements in indium selenide crystals.

We carried out the calculations of the band spectrum, the partial density densities and the spatial distribution of the valence electron density for a β -InSe crystal with different concentrations of transition metal impurities (Mn, Ni, Co). The evolution of spin-polarized spectra and partial charge densities for spin subsystems in diluted magnetic impurities of indium selenides has been analyzed. We found that diamagnetic structures of β -InSe and γ -InSe after intercalation with 3d elements become magnetically ordered. The estimates for the magnetic moment and their dependence on the concentration of impurities are obtained. It is shown that the local magnetic moment for Mn is greater than that for Ni and Co atoms. The decreasing of the magnetic moment of the impurity atoms in the In-Se layered crystals in a result of their intercalation by the transition metal atoms is observed too. The nature of the ferromagnetic order in intercalated β -InSe crystals is determined, due to the hybridization of the d-states of the impurity with the p-states of the chalcogen.

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Flexo-chemical coupling in ferroelectric thin films with defect layer

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We considered the impact of the flexoelectro-chemical coupling on the size effects in polar properties and phase transitions of thin ferroelectric films with a layer of elastic defects. A typical case is considered, when defects fill a thin layer below the top film surface with a constant concentration creating an additional gradient of elastic fields.

Obtained results revealed an unexpectedly strong effect of the joint action of Vegard stresses(W) and flexo-chemical coupling on the ferroelectric transition temperature, distribution of the spontaneous polarization and elastic fields, domain wall structure and period in thin PbTiO3 films containing a layer of elastic defects. A nontrivial result is the ferroelectricity persisting at film thicknesses below 4 nm, temperatures lower than 350 K and relatively high surface screening length (0.1 nm).

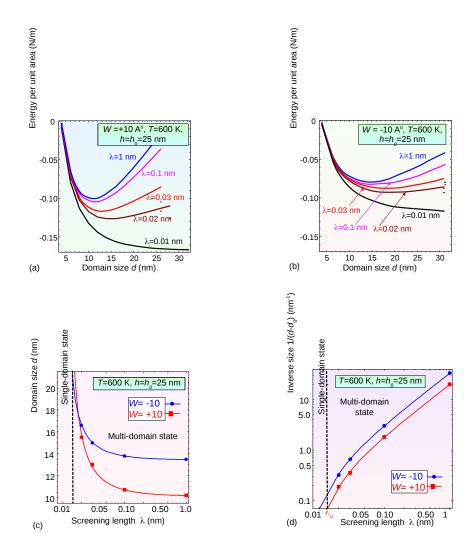


Figure 3 (a) (b) The dependence of the 25-nm thick $PbTiO_3$ film total energy on the domain size (potential relief of wall-wall interaction) calculated for different values of surface screening length λ , for different Vegard coefficient. Dependences of the equilibrium domain size (c) and inverse value (d) on the surface screening length λ . Temperature T = 600K and defect concentration $N_0 = 3 \times 10^{26} m^{-3}$.

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The bias error of flicker noise spectral exponent estimation

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Flicker noise (or 1/f noise) widespread in nature and has power spectral density $G(f) \sim 1/f^{\gamma}$, where f is the frequency, γ is the spectral exponent [1]. Spectral exponent is often used for reliability estimation of semiconductor devices. In [2] it is supposed, that the spectral exponent is function of f. When we have deal with real noise we may measure $\gamma(f)$ as a piecewise-defined function. Then spectral exponent relative bias error [3, 4] for some f_0 is

$$\delta_{\gamma} = \frac{1}{\gamma \cdot \ln\left(\frac{f_0 + \frac{\Delta f_{rel}}{2}}{f_0 - \frac{\Delta f_{rel}}{2}}\right)} \ln\left[\frac{24 + \gamma \cdot (\gamma + 1) \cdot \frac{\Delta f_{rel}^2}{\left(f_0 - \frac{\Delta f_{rel}}{2}\right)^2}}{24 + \gamma \cdot (\gamma + 1) \cdot \frac{\Delta f_{rel}^2}{\left(f_0 + \frac{\Delta f_{rel}}{2}\right)^2}}\right],\tag{1}$$

where f_0 is the central frequency, Δf_{rel} is the relative bandwidth for spectral exponent estimation.

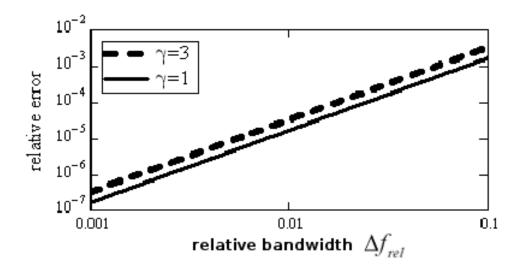


Figure 4 Dependence of bias error on relative bandwidth for spectral exponent.

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Dielectric properties of nanocellulose aqueous suspension

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We investigated dielectric properties of cellulose nanocrystals (CNC) and nanofibers (CNF) aqueous solutions. Mesurements of complex dielectric relaxation were performed in range of frequences from 10^9 to $2*10^{10}$ Hz. This range of frequences represents characteristics of hydrogen bonds. Using Debye theory, temperature dependence of characteristic relaxation time τ was determined for water, water-CNF suspension and water-CNC suspension (Fig.1). For water-CNC suspension charachteristic relaxation time is less than for water or water-CNF solution. This result we explain by properties of CNC, exactly, by its level of hydrophylity. Majority of molecules slowing dynamics of water, but some researches show that in some cases hydrophilic surface may faster water dynamics [1,2].

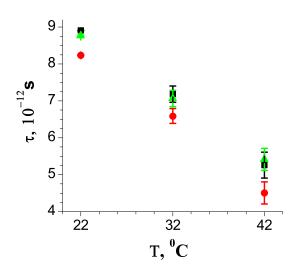


Figure 5 Characteristic relaxation time τ of \blacksquare water, \blacktriangle water-CNF, \blacklozenge water-CNC solutions.

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Stabilization of magnetic skyrmions by RKKY interactions

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We study the stabilization of an isolated magnetic skyrmion in a magnetic monolayer on non-magnetic conducting substrate via the Ruderman-Kittel-Kasuya-Yosida (RKKY) exchange interaction. Two different types of the substrate are considered, usual normal metal and single-layer graphene. We show that a proper treatment of the long-range RKKY interaction leads to a qualitatively different scenario compared to previous studies, where solitons were stabilized by the frustrated exchange coupling (leading to terms with the fourth power of the magnetization gradients [1]) or by the Dzyaloshinskii-Moriya interaction (described by terms linear in the magnetization gradients [2], [3], [4]). We exploit the fact that main part of the energy is R-independent, and thus the stabilization is driven by weak interactions which can be treated perturbatively as small corrections. We obtained that the RKKY exchange interaction results in a negative contribution to the skyrmion energy of the type $-(R/a)^{\alpha}$ with $0 < \alpha \le 1$. Combined with the contribution of the easy-axis anisotropy which is positive and proportional to $(R/a)^2$, this provides a novel mechanism of the skyrmion stabilization. In the case of a metallic substrate, we find that the skyrmion stabilization is possible under restrictive requirements on the Fermi surface parameters, and the RKKY contribution is non-analytic $(\alpha = \frac{1}{2})$. In the case of a graphene substrate $\alpha = 1$, the stabilization is naturally achieved in several geometries.

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Physics of Nuclei and Elementary Particles

The liquid droplet view on the phase transition in SU(2) gluodynamics

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The liquid droplet formula is applied to an analysis of the properties of geometrical (anti)clusters formed in SU(2) gluodynamics by the Polyakov loops of the same sign. Using this approach, we explain the phase transition in SU(2) gluodynamics as a transition between two liquids during which one of the liquid droplets (the largest cluster of a certain Polyakov loop sign) experiences a condensation, while the droplet of another liquid (the next to the largest cluster of the opposite sign of Polyakov loop) evaporates. The clusters of smaller sizes form two accompanying gases, which behave oppositely to their liquids. The liquid droplet formula is used to analyze the size distributions of the gaseous (anti)clusters. The fit of these distributions allows us to extract the temperature dependence of surface tension and the value of Fisher topological exponent τ for both kinds of gaseous clusters. It is shown that the surface tension coefficient of gaseous (anti)clusters can serve as an order parameter of the deconfinement phase transition in SU(2) gluodynamics. The Fisher topological exponent τ of clusters and anticlusters is found to have the same value 1.806 ± 0.008 . This value disagrees with the famous Fisher droplet model, but it agrees well with an exactly solvable model of the nuclear liquid-gas phase transition. This finding may evidence for the fact that the SU(2) gluodynamics and this exactly solvable model of nuclear liquid-gas phase transition are in the same universality class

Quantum van der Waals model versus Walecka model of nuclear matter ${\bf R.V.\ Poberezhnyuk}$

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A comparable study of the quantum van der Waals and Walecka models of nuclear matter is presented. Each model contains two parameters which characterize the repulsive and attractive interactions between nucleons. These parameters are fixed in order to reproduce the known properties of the nuclear ground state. Both models predict a first-order liquid-gas phase transition and a very similar behavior in the vicinity of the critical point. Critical exponents of the quantum van der Waals model are studied both analytically and numerically. There are important differences in the behavior of the thermodynamical functions of the considered models at large values of the nucleon number density. At the same time both models fall into the universality class of mean-field theory.

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Color structure of magnetic mass of chromomagnetic field

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Color structure of gluon field magnetic mass is investigated by means of lattice SU(2) gluodynamics at deconfinement phase.

Two external chromomagnetic fields are introduced on a lattice: the field of monopole-antimonopole string and the homogeneous Abelian field. In the first one all the SU(2) components are non-zero, while the Abelian field corresponds just to the diagonal generator of the SU(2) group.

The influence of the external Abelian field on the magnetic mass of the field of the monopole-antimonopole string is investigated. Three situations are considered:

- when the external Abelian field is absent;
- when the external Abelian field is parallel to the string;
- when the external Abelian field is perpendicular to the string.

It is shown that addition of the Abelian field does not change the magnetic mass of the string field. This means that the magnetic mass of the Abelian chromomagnetic field is zero and that the magnetic mass of the field of the monopole-antimonopole string is produced by its non-Abelian components. The first conclusion is consistent with other analytical and lattice investigations [1, 2], while the second statement was not investigated on the lattice before and is consistent with perturbative results [3].

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Electroweak phase transition in a spontaneously magnetized vacuum

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Chromomagnetic fields B_3 and B_8 have to be created spontaneously in the gluon sector of QCD at temperature $T > T_d$ higher the deconfinement temperature $T_d[1]$. Usual magnetic field H should also be spontaneously generated in the electroweak sector of the standard model at temperatures $T > T_{ew}$ higher than electroweak phase transition temperature T_{ew} [2]. Quarks possess both electric e and color g charges. So, due to vacuum polarization, the mixing of classical color and usual magnetic fields happens. In the temperature interval $T_d < T < T_{ew}$ the color fields in an effective potential act as specific sources for H [3]. The field strengths are estimated to be of the order B_3 , $B_8 \sim 10^{18} - 10^{19}G$, $H \sim 10^{16} - 10^{17}G$ for temperatures $T \sim 160 - 220 MeV$.

We investigate the electroweak phase transition in the One-Higgs-Doublet and Two-Higgs-Doublet standard models with accounting for the spontaneous vacuum magnetization. Already such type considerations have been done as a problem in different type given external magnetic fields. Since the spontaneously generated fields are temperature dependent and strong they influence essentially the phase transition. We determine the mass interval for Higgs particle when the phase transition is strong first order and fits Sakharov's conditions for the formation of the baryon asymmetry of the Universe. The field strengths $B_3(T)$, $B_8(T)$ and H(T) at relevant temperatures are also estimated.

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Cumulative production of nucleons by heavy baryonic resonances in proton-nucleus collisions

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I investigate nucleon production in proton-nucleus collisions outside the kinematical boundary of proton-nucleon reactions. The maximal energy of protons emitted in the backward direction is estimated. I suggest that cumulative nucleons are produced by heavy baryonic resonances created in p+A collisions due to successive collisions with nuclear nucleons. I also compare theoretical predictions to the results of Ultrarelativistic Quantum Molecular Dynamics simulations.

Possibility of the Abelian Z' with a non-narrow resonance within the model-independent approach

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The Abelian Z' boson is investigated in a model-independent approach [1]. In the framework of the specific Z' models, the Z' mass is the only free parameter that must be fitted. In the model-independent approach, it becomes possible to estimate the Z' couplings to the SM fields independently. We start from the effective Lagrangian of the Z/Z' interaction with the SM fermions:

$$L_{Z\bar{f}f} = \bar{f}\gamma^{\mu} \left[\left(v_f^{SM} + \gamma^5 a_f^{SM} \right) \cos \theta_0 + \left(v_f + \gamma^5 a_f \right) \sin \theta_0 \right] f Z_{\mu} / 2, \tag{6}$$

$$\mathcal{L}_{Z'\bar{f}f} = \bar{f}\gamma^{\mu} \left[\left(v_f + \gamma^5 a_f \right) \cos \theta_0 - \left(v_f^{SM} + \gamma^5 a_f^{SM} \right) \sin \theta_0 \right] f Z'_{\mu} / 2, \tag{7}$$

where θ_0 is the Z-Z' mixing angle. We assume that 1) the Z' mass is acquired through the Higgs mechanism; 2) the theory is renormalizable; and 3) the axial-vector couplings are universal, so that $a=a_e=-a_{\nu_e}=a_d=-a_u$. Hence, the following relations appear between the Z' parameters:

$$v_f - a_f = v_{f_*} - a_{f_*}, \quad \theta_0 = -2a\alpha_{em}^{-1/2}\sin\theta_W\cos\theta_W(m_Z/m_{Z'}) + O((m_Z/m_{Z'})^4),$$
 (8)

where f and f_* are the partners of the $SU(2)_L$ fermion doublet, α_{em} is the fine structure constant, θ_W is the Weinberg angle. Therefore, only four Z' parameters stay independent, for example, a, v_e , v_u , and $m_{Z'}$.

Provided that the Z-Z' mixing takes place, the Z' couplings can modify observables for the Z. In particular, we discuss the total Z decay width. The current experimental constraints on it are $\Gamma_Z = 2.4952 \pm 0.0023$ GeV. Thus, we can restrict the Z' parameters in order to make Γ_Z stay within these limits. Using (6) and (7), we obtain the optimistic estimate for the universal axial-vector coupling a:

$$|\bar{a}| < 0.02, \quad \bar{a} \equiv (4\pi)^{-1/2} (m_Z/m_{Z'}) a.$$
 (9)

This restriction allows also to constrain the Z' decay width. With (9), we obtain

$$\Gamma_{Z'}/m_{Z'} < 30\%.$$
 (10)

We hereby see that the non-narrow Z' resonances are allowed. This is the main result of the present work which agrees with the recent known results [2].

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| 5 | Odesa State Environmental University, Odesa |
| 6 | Institute for Problems of Materials Science, NAS of Ukraine, Kyiv |
| 7 | Institute for Single Crystals of NAS of Ukraine, Kharkiv |
| 8 | National Mining University, Dnipro |
| 9 | Taras Shevchenko National University of Kyiv |
| 10 | Oles Honchar Dnipropetrovsk National University, Dnipro |
| 11 | Ivan Franko National University of Lviv |
| 12 | Uzhhorod National University, Institute of Physics and Chemistry |
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| 13 | Lesya Ukrainka Eastern European National University, Lutsk |
| 14 | Ulyanovsk State Technical University, Ulyanovsk, Russia |