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## **Book of Abstracts**

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## Statistical Theory of Many-body Systems

# Linear-in-gradients hydrodynamic equations for a system with small interaction

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The system under consideration is a one-component weakly non-uniform gas with small potential interaction. The investigation is based on the kinetic equation in the case of small interaction with a nonlocal collision integral [1]. In [2] it is shown that the system kinetic energy is not conserved on the basis of the nonlocal collision integral. So the system temperature should be defined on the basis on the total system energy rather than the kinetic one. The following hydrodynamic equations are obtained up to the first order in small gradients and the second order in small interaction:

$$\begin{aligned}\frac{\partial n}{\partial t} &= -n \frac{\partial v_n}{\partial x_n} - v_n \frac{\partial n}{\partial x_n}, \quad \frac{\partial v_n}{\partial t} = -v_l \frac{\partial v_n}{\partial x_l} + \left[ -\frac{T}{nm} - \frac{1}{m} V(k=0) + \right. \\ &+ \left. \frac{1}{2\pi^2 m T} \left( A + \frac{B}{3} \right) \right] \frac{\partial n}{\partial x_n} + \left[ -\frac{1}{m} - \frac{n}{4\pi^2 m T^2} \left( A + \frac{B}{3} \right) \right] \frac{\partial T}{\partial x_n}, \\ \frac{\partial T}{\partial t} &= \left[ -\frac{2}{3} T + \frac{n}{9\pi^2 T} \left( A + \frac{B}{2} \right) \right] \frac{\partial v_n}{\partial x_n} - v_n \frac{\partial T}{\partial x_n}, \\ A &= \int_0^\infty dk k^2 V^2(k), \quad B = \int_0^\infty dk k^3 V(k) \frac{\partial V(k)}{\partial k}\end{aligned}$$

where  $n$  is the particle number density,  $v_l$  is the velocity,  $T$  is the temperature, and  $V(k)$  is the Fourier transform of the system pair potential. In fact, these equations are non-dissipative hydrodynamic equations and in the leading-in-interaction order they coincide with corresponding equations in the framework of standard hydrodynamics. The obtained equations may be a basis for the investigation of the system dissipative hydrodynamics and system kinetic coefficients.

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

[2] V.N. Gorev and A.I. Sokolovsky, *Visnik Dnipropetrovs'kogo Universitetu. Seria Fizika, radioelektronika*, 25, issue 24, 14 (2017).

## Statistical Theory of Many-body Systems

# Towards the problem of the Nesterenko's soliton waves propagation in nonlinear inhomogeneous Hertzian chains

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We consider theoretically the problem of the pulse transmission along 1D vertical chain of hard spheres, which interact with each other by pair-wise nonlinear Hertz law [1-3]. System is subject into gravity and therefore became inhomogeneous [2,3]. We show, that being excited from the boundary (from the top), system is able to exhibit complex multimode dynamics of pulse propagation. After long-wave approximation has been used to study the dynamics of weak perturbation, in the lowest approximation, resulted governing equation is satisfied by either singular solutions, or combinations of cylindrical waves [2]. In the higher approximation we obtain nonlinear equation of motion (generalized in form of Boussinesq equation) which brings us to solution of Nesterenko-type soliton [1] with negligible differences in the amplitudes, and dispersions.

We conclude that initially weakly nonlinear and inhomogeneous chain, already in the linear approximation, is able to transmit either normal or singular modes, whenever, the accounting, of the nonlinearity leads to familiar Nesterenko-type soliton's [1].

Therefore under the appropriate values of the parameters (nonlinearity, inhomogeneity, signal amplitudes) linearized Hertzian chain support both discontinuous as well as quasinormal mode scenarios of pulse transmission.

[1] Nesterenko, V.F. Propagation of nonlinear compression pulses in granular media. *J. Appl. Mech. Tech. Phys.* 24 (1) (1984) 733-743; Translated from : *Zh. Prikl. Mekh. Tekh. Fiz.* (5) (1983) 136-148. [Russian]

[2] Sen, S., Hong, J., Bang, J., Avalos, E., and Doney, R. Solitary waves in the granular chain. *Physics Reports* 462 (2) (2008) 21-66.

[3] Gerasymov, O.I. and Vandewalle, N. On the exact solutions of the problem of impulsive propagation in an inhomogeneous granular chain. *Dopov. Nac. acad. nauk Ukr.* (8) (2012) 67-72. [Ukrainian]

## Statistical Theory of Many-body Systems

# The influence of inhomogeneities on physical characteristics of ferromagnetic clusters inside of antiferromagnetic matrix in an external field

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The problem of the influence of an external field on the magnetic moments of ferromagnetic clusters surrounded by an antiferromagnet is studied in this paper. Clusters interact with each other magnetically. In the case of strong anisotropy such a system can be described by a one-dimensional Ising model with a random exchange in the presence of an effective local field. The inhomogeneity of the interface between clusters and an antiferromagnet represents the random effective field. The ground state of such a model turns out to be the set of domains of different lengths in fields smaller than the saturation field. In contrast to the one-dimensional Ising model in a homogeneous field, linear dependence of the magnetization on the external field in the presence of a random effective field in the region of small fields is observed. The magnitude of the exchange bias of the magnetization curve depends on the average of the random effective field, and the slope of the curve depends on the variance of the random effective field. The use of such a model allows drawing conclusions about the properties of the boundary between subsystems from experimental data. The results obtained within the framework of such model allow to estimate the properties of the boundary between subsystems basing on experimental data. A formula that estimates the quality of the interface in the case of the cylindrical geometry of the sample is obtained.

## Statistical Theory of Many-body Systems

# Calculation of thermodynamic potential for Bose system near condensate point

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Bose system in the presence of the 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  $p = 0$  is macroscopic one. In this model the system is described by the statistical operator

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

where operators  $\hat{H}(n_0)$ ,  $\hat{N}(n_0)$  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  $a_0, a_0^+$  ( $\beta, \mu$  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 non-equilibrium one of the system. Near transition point from normal state to the state with the condensate occupation number  $n_0$  is small in comparison with the total number of particles 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 statistical operator  $w(n_0)$  can be written in the form  $w(n_0) = \exp \beta [F - (\hat{\mathbf{H}}_0 + \hat{U}_1 + \hat{U}_2)]$  where the operators  $\hat{U}_1 \sim n_0^{1/2}, \hat{U}_2 \sim n_0$ . The calculation is substantially simplified by the fact that the independent on  $n_0$  operator  $\hat{\mathbf{H}}_0$  commutes with the operator of the number of particles. It is shown that only integer powers of this number are present in expansion of the potential. Relatively compact expressions for the coefficients of this series are obtained because operators describing the interaction in the system commute under T-product. For a Bose gas they are calculated in an additional perturbation theory in interaction between particles. An analyze of the results with connection to the Landau theory of phase transitions is given.

[1] Akhiezer, A.I. Methods of Statistical Physics [Text] / A.I. Akhiezer, A.I. and S.V. Peletminskii. – Oxford: Pergamon Press, 1981. – 450 p.



## Statistical Theory of Many-body Systems

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

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We consider a class of spiking neuronal models with threshold 2, 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 Poisson process. Each output impulse is applied to the neuron itself after a finite delay  $\Delta$ . This impulse is identical to those delivered from the input stream. 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, intensity of the input stream and the properties of the feedback line (the  $\Delta$  value).

In addition to this, we calculate exactly the model-independent initial segment of pdf  $p(t)$  for a neuron with feedback that is the same for any neuron satisfying the imposed conditions. Also, relations between moments of pdf  $p(t)$  for a neuron with feedback and pdf  $p^0(t)$  for the same neuron without feedback are derived. The obtained expressions are checked numerically by means of Monte Carlo simulation.

The course of  $p(t)$  has a  $\delta$ -function peculiarity, which makes it impossible to approximate  $p(t)$  by Poisson or another simple stochastic process.

## Physics of Biological Macromolecules

# Blocking of DNA sites of specific recognition by hydrogen peroxide molecules in the process of ion beam therapy

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After irradiation of cancer cells in the ion beam therapy method the concentration of hydrogen peroxide in the cell medium grows significantly. But the role of hydrogen peroxide molecules in ion beam therapy has not been determined yet. We assume that interaction of peroxide molecules with DNA atomic groups can block the genetic information of the cancer cell and lead to its neutralization. To understand the possibility of DNA deactivation in the cell, in the present study the formation of complexes of hydrogen peroxide with DNA specific recognition atomic groups is considered. Using atom-atom potential functions method and quantum-chemical approach, based on density functional theory, the spatial configurations and energy minima for the complexes of peroxide and water molecules with nucleic bases are studied. The obtained data allows us to formulate a new, different from the already known, mechanism of the ion irradiation action on living cells, that can be the key factor in the ion beam therapy treatment.

## Physics of Biological Macromolecules

# Atomic charges for reproducing the dependence of molecular dipole moment on conformation

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A modification of the principal component regression model is proposed for obtaining a fixed set of atomic charges (referred to as dipole-derived charges) optimized for reproducing the dipole moment of a conformationally rich molecule, i.e., a molecule with multiple local minima on the potential energy surface. The method requires geometry of the conformers, their dipole moments and APT charges (which only depend on the derivatives of the dipole moments with respect to the atomic coordinates) in each of the conformers as input data, and produces a single set of fixed charges suitable for accurate representation of both the dipole moment vector of all conformers and its variations resulting from small changes in molecular geometry (e.g., caused by vibrations) [1]. The peculiar feature of the method is that it requires neither adjustable empirical parameters, nor averaging over conformers or any other post-processing of the obtained charges. The input data used in the proposed method are obtained from ab initio calculations which also do not require empirical parameters.

The proposed method has been applied to canonical 2'-deoxyribonucleotides, the model DNA monomers, and the dipole-derived charges have been shown to outperform both the averaged APT and RESP charges in reproducing the dipole moments of large sets of conformers, thus demonstrating a potential usefulness of the dipole-derived charges as a 'reference point' for modeling polarization effects in conformationally rich molecules, parameterizing non-polarizable force fields and for developing novel polarizable force fields for classical MD simulations.

[1] T.Yu.Nikolaienko and L.A.Bulavin, Phys. Chem. Chem. Phys, 20, 2890-2903 (2018).

## Physics of Biological Macromolecules

# Modeling of activation and deactivation processes in postsynaptic membrane

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Modern technologies are increasingly turning to the issue of modeling nerve impulse transmission mechanisms to create artificial simulators. Despite the fact that the basic principles of the specialized contact zone between two neurons (chemical synapse) are known, there still a lot questions are open.

In this paper, we research the issue of building a physical model of the process of activation and deactivation of the postsynaptic membrane in a chemical synapse. Based on the diffusion process, considering the interaction of choline with receptors on the postsynaptic membrane, we obtained a temporary dependence of activated receptors on the postsynaptic membrane. The relationship between the activation time of the postsynaptic membrane and the number of activated receptors was also analyzed. The work also calculated the space-time distribution of the anti - mediator (choline) in the synaptic cleft.

We hope that the results obtained in the work will help to better understand the processes occurring during the transmission of the nerve signal and will give impetus to further research in the field of medical preparations and the construction of artificial neural networks.

**Astrophysics and Cosmology**

# **Reconstructed potentials of the 2-field model of dark energy with canonical and non-canonical kinetic terms**

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We generalize quintom to include the tachyonic kinetic term along with the classical one. For the spatially flat, homogeneous and isotropic Universe with Friedmann-Robertson-Walker metric of 4-space we discuss in detail the reconstruction of the scalar fields potential  $U(\phi, \xi)$ . Such a reconstruction cannot be done unambiguously, so we consider 3 simplest forms of  $U(\phi, \xi)$ : the product of  $\Phi(\phi)$  and  $\Xi(\xi)$ , the sum of  $\Phi(\phi)$  and  $\Xi(\xi)$  and this sum to the  $\kappa$ th power. We present the maps of reconstructed potentials for the Chevallier-Polarski-Linder parametrization of the equation of state parameter and the set of cosmological parameters obtained from the latest Planck data.

**Astrophysics and Cosmology**

## **The 3.5 keV dark matter candidate line in the Galactic bulge region**

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The 3.5 keV line, discovered in early 2014 in the spectra of different cosmic objects, draws large attention as being the dark matter signal candidate. Much effort was performed since then to determine it's nature. The one conclusion to point out is that the dark matter signal is by now the only explanation consistent with all the observational data available.

We are presenting the detection of the 3.5 keV line in the stacked spectra of the XMM-Newton observation of the Galactic bulge region. The line was detected significantly in the several annulus regions around Galactic center. Being interpreted as dark matter decay line, this allows us to determine the inner halo profile slope.

We also briefly discuss the perspectives of the planned experiments in frames of our restrictions on signal parameters.

## Astrophysics and Cosmology

# 21-cm observations and warm dark matter models

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Recent report of 21-cm absorption signal by EDGES experiment has raised considerable interest in the dark matter (DM) community. Taking the reported EDGES result at face value, a number of forthcoming papers constrained masses of DM particles and their interaction strengths with Standard Model particles.

However, the connection between the formation of structures and 21-cm signal requires knowledge of parameters that describe star formation and radiation at early times.

We use the recent measurements by EDGES to demonstrate that the robust warm dark matter (WDM) bounds are in fact weaker than those given by the Lyman- $\alpha$  forest method and other structure formation bounds.

We also show that resonantly produced 7 keV sterile neutrino dark matter model is consistent with these data.

## Astrophysics and Cosmology

# Constraints on the excess energy in low-mass systems

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We present the  $K - T$  scaling relation of the individual galaxies (mostly early-type galaxies), groups, and clusters. The given relation is based on 168 targets observed with *Chandra* X-ray Observatory. We derive entropy at  $R_{2500}$  and build  $K_{2500} - T$  relation covering 0.3 – 15.0 keV of temperature and  $10^{12} - 10^{15} M_{\odot}$  of total mass bands. We find that entropy at  $R_{2500}$  scales with averaged temperature as  $K_{2500} \propto T^{0.68 \pm 0.05}$ , leading to the break of a self-similar model. We compare our measurements with previous results and find precise agreement with  $K - T$  relations obtained for entropies at  $R_{200}$  and  $R_{500}$  radii. The break of the self-similar model indicates the presence of non-gravitational processes at the cores of low- and high-mass systems which provide an additional heating that is known as entropy excess in  $K - T$  relation. We show that AGN feedback is likely mechanism producing this additional heating. We also show that active nuclei in low-mass systems are better able to prevent the significant level of star formation due to enough cooling nearby the nucleus to maintain the energetic feedback loop by measuring the level of heating per gas particle in hot atmospheres of low- and high-mass systems. In addition, using radio flux and luminosity we build the entropy-cavity power relation, finding a weak correlation of  $K_{2500} \propto P_{cav}^{0.25 \pm 0.5}$ .



## Astrophysics and Cosmology

# $\mu$ -Bose-Einstein condensate dark matter model

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It is known that the Bose-Einstein condensate (BEC) based Dark Matter (DM) model solves several problems of Cold Dark Matter model on the small scales, including core-cusp problem. In turn, there are some difficulties that arise in the framework of BEC DM, like overestimated a bit (up to 20%) prediction of halo mass in comparison with the values derived from observations. In ref. [1], the extended (via  $\mu$ -deformation)  $\mu$ -BEC DM model is proposed. The  $\mu$ -deformed gas has the properties similar to ordinary Bose gas endowed with an additional attraction between its particles, incorporated [2] by the deformation parameter  $\mu$ . We prove the possibility of BEC-like phase transition using the tools of thermodynamical (Ruppeiner) geometry, through analysis of singularities of scalar curvature in the thermodynamical parameters space. It is shown that the critical temperature of BEC-like transition is higher in the considered  $\mu$ -Bose gas than in the ordinary Bose case. Moreover, dependence on the parameter  $\mu$  gives us certain freedom enabling to treat the weak points of BEC DM model, e.g. the overestimated value of DM halo mass.

- [1] A.M. Gavrilik, I.I. Kachurik, M.V. Khelashvili, A.V. Nazarenko Condensate of  $\mu$ -Bose gas as a model of dark matter. *Physica A*: V.506, pp. 835-843 (2018)  
[2] A.P. Rebesh, I.I. Kachurik, A.M. Gavrilik Elements of  $\mu$ -calculus and thermodynamics of  $\mu$ -Bose gas model, *Ukr. J. Phys.* V. 58, no.12, pp. 1182-1191 (2013)

## Condensed Matter Physics

# Equilibrium states of antiferromagnetic ring-shaped and helix-shaped spin chains with hard-tangential anisotropy

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For the last decade, active research on magnetic nanosystems of curved geometry was motivated by their outstanding properties and great application potential [1]. For instance, recent theoretical studies of low-dimensional magnets with complex geometry propose a description of fascinating geometry-induced effects including pattern formation and magnetochiral effects in quasi-one-dimensional wires [2], for review see [1]. Despite these advances in the study of curvilinear low-dimensional ferromagnets, significant knowledge gaps exist in the study of curvilinear antiferromagnetic systems.

The purpose of the current study is the theoretical investigation of equilibrium states in antiferromagnetic ring-shaped and helix-shaped spin chains with hard-tangential anisotropy. For this purpose we use both analytical methods and computer spin-lattice simulations in SLaSi software package [3]. In our study, we consider two sublattice antiferromagnet in the frame of the sigma-model approach where its statics and dynamics are described in terms of Neel vector only.

We analytically show that the global energy minimum of the antiferromagnetic ring-shaped spin chain is reached when Neel vector is perpendicular to the ring plane. An equilibrium phase diagram is constructed for the antiferromagnetic helix-shaped spin chain: (i) a quasi-binormal state is realized in the case of relatively large curvatures and (ii) spatial-periodic state is typical in the opposite case. Both states are described analytically and well confirmed by SLaSi.

Stability regions of both ground states are determined using spin-lattice simulator SLaSi.

[1] R. Streubel, P. Fischer, F. Kronast, V. P. Kravchuk, D. D. Sheka, Y. Gaididei, O. G. Schmidt and D. Makarov, *J. Phys. D*, 49, 363001, (2016).

[2] D. D. Sheka, V. P. Kravchuk, Y. Gaididei, *J. Phys. A*, 48, 125202, (2015).

[3] <http://slasi.knu.ua/>

## Condensed Matter Physics

# An effective theory for Heisenberg antiferromagnet on one-dimensional frustrated lattices at high magnetic fields

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We consider the spin-1/2 antiferromagnetic Heisenberg model on one-dimensional frustrated lattices (double tetrahedra chain [1], deformed octahedral chain [2]) placed in an external magnetic field with almost dispersionless (almost flat) lowest magnon band. The main goal of our study is to develop a systematic theory for the low-temperature high-field properties of these models, using the localized magnons approach [3,4]. We construct an effective description of one-dimensional chains with triangular and quadrangular traps by means of the localized magnons concept within the strong coupling approximation. The obtained effective models are much simpler than the initial ones: firstly, the effective models have smaller number of sites and secondly, and most importantly, they are unfrustrated. As a result, one can apply well elaborated methods of the quantum spin systems theory to discuss the properties of the initial frustrated quantum antiferromagnets at high fields and low temperatures. We perform extensive exact diagonalization calculations to check the validity of the obtained effective Hamiltonians by comparison with the initial models.

[1] M. Maksymenko, O. Derzhko and J. Richter, *Acta Physica Polonica A* **119**, 860 (2011); *Eur. Phys. J. B* **84**, 397 (2011).

[2] J. Strečka et al., *Phys. Rev. B* **95**, 224415 (2017); *Physica B* **536**, 364 (2018).

[3] J. Schulenburg et al., *Phys. Rev. Lett.* **88**, 167207 (2002).

[4] O. Derzhko, J. Richter, and M. Maksymenko, *Int. J. Mod. Phys. B* **29**, 1530007 (2015).

**Condensed Matter Physics**

# **Ground-state phases of frustrated bilayer quantum Heisenberg antiferromagnets**

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We consider the quantum antiferromagnetic Heisenberg model on the square-lattice and honeycomb-lattice bilayers in the absence of an external magnetic field. We use a variational approach to construct the ground-state phase diagrams of such model on different bilayers. For simplicity, we choose two one-parameter variational wave functions, which can describe states of model in two regions with different relationships between lattice parameters. We calculate variational energies and compare them. This allows us to find borders between different states, where one of the variational energies is minimal. Finally, we construct ground-state phase diagrams in different coordinates. At the end of this study we compare our findings with the earlier results obtained by more sophisticated approaches [1, 2]. We observe good agreement with these results. This studies were performed together with O. Derzhko, J. Richter and O. Götze.

[1] H. Zhang et al., Phys. Rev. B 93, 235150 (2016);

[2] J. Stapmanns et al., Phys. Rev. Lett. 121, 127201 (2018).

## Condensed Matter Physics

# Boundary conditions for the superconducting junctions at temperatures close to critical

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To calculate the current-phase relation in superconducting junctions, it is necessary to investigate the spatial behavior of the order parameter in the superconducting regions of the junction. In the case of temperatures close to the critical one, the Ginzburg-Landau theory [1] is used for this purpose. However, to apply this theory there is necessary to find the corresponding boundary conditions for the Ginzburg-Landau equation. Boundary condition can be found using the Wiener-Hopf method [2-3], however, use of this method for complicated superconducting junctions is problematic.

In our investigation, the problem of finding boundary conditions for the Ginzburg-Landau equation, was considered in the case of different superconducting junctions. In particular, superconducting junctions, combining tunnel effects and the proximity effect, with nonmagnetic impurities in superconducting regions were investigated. For finding the boundary condition for the Ginzburg-Landau equation the method of quasiorthogonality to asymptotics was used [4]. In addition, there were no restrictions on the values of the electron transmission coefficient and the thickness of the normal layer.

It has been shown that the boundary condition for the Ginzburg-Landau equation contains unknown constants for the calculation of which the quasiorthogonality to the asymptotics method was used. This method proved to be quite effective for complicated superconducting systems which contain the combination of dielectric layer and normal layer. In addition, boundary conditions obtained using this method, are valid for the arbitrary concentration of non-magnetic impurities.

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## Condensed Matter Physics

# A current density dependence on phase differences in layered superconducting structures of SISIS type

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The explored layered superconducting structure contains three massive superconductors separated by two thin insulator films. Without loss of generality we may consider that the superconductors are different. An insulator film is mathematically expressed via the Dirac delta function [1]. An order parameter and a current density depend on an applicate, because we have a one dimensional problem.

According to the superconductivity theory every physical quantity can be calculated using the Green function method [2]. The Green functions satisfy the closed system of linear differential equations. The mentioned equations have the second derivative in the configuration representation. Using the Fourier transform we have constructed the closed system of linear matrix differential equations in the  $t$ -representation [3]. The obtained equations have only the first derivative. Since a momentum is close to the Fermi momentum our calculations become rather simplified. Solving the linear matrix differential equations in the  $t$ -representation we have introduced the undefined integration constants. These constants can be defined through application of Green function continuity. This means that we need to have a boundary condition. An order parameter as a complex function is usually defined by magnitude and phase. The model with a piecewise constant order parameter allows to suppose that the outside superconductors have equal order parameter magnitudes and unequal order parameter phases. The inside superconductor has a zero order parameter phase. The order parameter magnitude of the inside superconductor is not necessary equal to the order parameter magnitudes of the outside superconductors.

Substituting the obtained integration constants into the Green functions we have obtained the current density dependence on an applicate. Calculating the current density on the junction we have obtained the current density expression as a phase difference function.

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## Condensed Matter Physics

# The third sound as an electric field generator

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It is predicted that oscillations of temperature during propagation of third sound in a thin superfluid film cause appearance of an alternating electric field in the surrounding space, i.e. the third sound acts as a generator of the electric field [1].

As known, the helium atoms have no dipole, quadrupole and other multipole moments. The situation changes in the vicinity of the wall. Interaction of helium with the container walls leads to the emergence of a nonzero average dipole moment of the helium atoms directed along the normal to the wall. This leads to polarization of the film. Oscillations of its surface are accompanied by polarization oscillations, which cause the appearance of the electric fields over the film. Specificity of a superfluid film is associated with the ability to cause oscillations of the film surface by periodically heating the film boundary. As a result, due to the anomalously large thermomechanical effect, a small temperature difference  $\Delta T$  leads to large fluctuations in film height and electrical potential  $\Delta\varphi$ . It turns out that the differential thermal e.m.f.  $\Delta\varphi/\Delta T$  exceeds its value for typical metals. The predicted effect can be considered as an electrical analogue of the fountain effect.

Using the method of I.E. Dzyaloshinskii, the average electric field over the system "atom-solid" was calculated. It is shown that this electrical field is equivalent to the field of the dipole moment of the atom (induced by substrate) and its image. The polarization of the system, associated with its inhomogeneity (analogue of the flexoelectric effect), was also considered. It has been established that the flexoelectric effect leads only to a small renormalization of the dipole moment induced by the substrate. The equations describing the propagation of the third sound through the film have been solved. The effects of evaporation and condensation of helium atoms were taken into account. The relationship between oscillating parts of the height and temperature of the film was found for the low-temperature and high-temperature regions. For helium film covering a hollow cylinder on the outside or inside, an analytical expression for the electric field in space has been found. The coefficient of proportionality between the electric potential and the oscillating part of the film temperature (differential thermal e.m.f) was calculated.

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## Condensed Matter Physics

# Features of light coupling in low-loss 2D periodic structures supporting phonon polariton

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Understanding of light-matter interaction in a wide frequency range is an important fundamental problem with significant potential applied impacts. For instance, Plasmonics is a rapidly developing field at the boundary of physical optics and condensed matter physics with many prospective applications. However, the use of plasmons is limited from a practical point of view because their spectral signature is in the visible and near infrared region, where metals have strong absorption leading to high losses. From this point of view, the use of low-loss materials, like polar dielectrics, is promising. Particularly, in such materials surface phonon polaritons can be easily excited from the infrared to the terahertz frequencies resulting in a strong coupling of light and optical phonons in the crystal.

In this report, we studied features of light localization in low loss 2D periodic structures formed by a polar crystal. Specifically, we considered a periodic structure of silicon carbide nanodisks on a crystalline silicon substrate. We numerically solved Maxwell equations with appropriate boundary conditions. The strong dependence of phonon polariton spectral resonances with the period of the array was theoretically revealed. Furthermore, experimental reflectivity measurements on the fabricated structure confirmed these tendencies.

## Condensed Matter Physics

# Influence of correlated hopping on the optical conductivity spectra

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Optical conductivity spectra are studied for the Falicov-Kimball model with correlated hopping on the Bethe lattice. An expression for the current-current correlation function is derived using dynamical mean field theory. Besides, the Nyquist plots were built and used to distinguish different contributions in the optical conductivity spectra.

In the metallic phase without correlated hopping, both the current-current correlation function  $\chi(\Omega)$  and optical conductivity  $\sigma(\Omega)$  display Drude peak at low frequencies. The shape of Drude peak is described by the Debye relaxation equation

$$\chi_D(\Omega) = \chi_\infty + \frac{\chi_0 - \chi_\infty}{1 - \Omega\tau_D}$$

On the other hand in the presence of small correlated hopping, the shape of Drude peak deviates from the Debye relaxation peak, and an additional wide peak is observed on the optical conductivity spectra and on Nyquist plot when Fermi level is in the vicinity of the two particle resonance [1]. At larger values of the correlated hopping parameter, the density of states contains three bands [1] and the corresponding optical spectra and Nyquist plots display a more complicated shape with additional peaks. For the case of strong local correlations, the overall picture strongly depends on the doping level. For a small doping, when the chemical potential is placed in the wide lower Hubbard band the obtained results are much closer to the case of the doped Mott insulator without correlated hopping, whereas for a large doping, when the chemical potential is placed in the narrow upper Hubbard band, the spectral weight of the Drude peak is strongly reduced and it is separated by a gap from the charge-transfer peak.

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## Condensed Matter Physics

# On consistency of classical homogenization models for the permittivity of statistically homogeneous mixtures

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The standard effective-medium methods to electrodynamic homogenization of heterogeneous media can be divided into two classes: symmetrical and asymmetrical. They are assumed to be independent and applicable to different types of systems, making a basis for different further modifications that take into account specific features of a given system. Despite the fact that these modifications are able to restore experimental data rather well, various authors note that the basic assumptions behind the methods are not consistent.

The goal of this report is to scrutinize these two homogenization methods, their consistency, and ranges of validity. To obtain the most general results, a simple system of impenetrable dielectric balls embedded in a uniform host medium has been considered. For its analysis, a generalized differential scheme was developed for the effective quasistatic permittivity of macroscopically homogeneous and isotropic dielectric mixtures [1]. The scheme is based upon the compact group approach (CGA) [2] reformulated in a way that allows one to analyze the role of different contributions to the effective permittivity of the system and modify it for different system structures.

It is shown that within the CGA, the only physically consistent homogenization type is symmetrical effective-medium homogenization. Applicability of this approach to the core-shell model and the description of numerical and experimental data for conductivity of composite electrolytes was demonstrated in [3]. The asymmetrical (differential) homogenization type can be obtained by replacing the electromagnetic interaction between previously added constituents and those being added by the interaction of the latter with recursively formed effective medium. Under this assumption, each portion of inclusions has different polarization, and the previously added portions do not interact with the new ones. This can be valid only for narrow concentration ranges and low contrast constituents, even for the generalized versions of the original mixing rules, as can be proved using the Hashin-Shtrikman bounds. Therefore, the asymmetric approach is approximate in the long-wave limit, and one should be cautious when using the differential models since they can lead to unpredictable errors and wrong results.

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## Condensed Matter Physics

# Features of thermal transport in strained and compressed crystalline silicon

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Tuning of thermal properties of various materials is a key challenge in material research. First and foremost, such necessity arises because of continuous miniaturization of constitute components of various devises. As a result, issue connected with amelioration of heat management started to be more and more crucial. Therefore, any possibilities of increasing or reduction of thermal conductivity in semiconductor material are very important.

One of the possibilities for variation of thermal transport is the change of elastic properties of the media. Particularly, it is well-known that straining and compression of crystalline silicon lead to modification of heat conduction. However, one needs more physical insight regarding phonon transport for efficient manipulation of heat fluxes.

In our study, we consider thermal conductivity of strained and compressed silicon as a function of strain and temperature. We use ab-initio equilibrium molecular dynamics approach for evaluation of thermal conductivity. Additionally, we extracted phonon density of states and dispersion curves from molecular dynamics simulations. These data were utilized for direct calculations of thermal conductivity with the use of kinetic theory approach. Comparison of molecular dynamics simulation and direct approach allows us to decompose different factors affecting the thermal conductivity of strained/ compressed silicon.

**Mathematical Physics**

# **Physics of singular self-adjoint extensions of one-dimensional Dirac operator**

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We consider boundary conditions (self-adjoint extensions) corresponding to point-like interactions for one-dimensional Dirac operator. Taking the non-relativistic limit we show how all possible point-like interactions for one-dimensional Schrödinger operator of free spinless particle can be obtained from the Dirac Hamiltonian. In case of spin-1/2 we show that there are boundary conditions with spin-flop mechanism. We suggest the physical interpretation these point-like extensions in terms of the Rashba (spin-orbital) coupling.

**Mathematical Physics**

# Tumour growth model: Lie symmetries and exact solutions

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We examine the tumour growth model proposed in [1]. In the 2D case, the governing equations after some simplifications take the form

$$\begin{aligned} \alpha_t + (\alpha u^1)_x + (\alpha u^2)_y &= S(\alpha), \quad u_x^1 + u_y^2 = \nabla \cdot (D(\alpha)\nabla p), \\ \left[ (2 + \lambda)\alpha u_x^1 + \lambda\alpha u_y^2 \right]_x + \left[ \alpha u_y^1 + \alpha u_x^2 \right]_y &= p_x + (\alpha\Sigma(\alpha))_x, \\ \left[ \alpha u_y^1 + \alpha u_x^2 \right]_x + \left[ (2 + \lambda)\alpha u_y^2 + \lambda\alpha u_x^1 \right]_y &= p_y + (\alpha\Sigma(\alpha))_y, \end{aligned} \quad (1)$$

where  $D$ ,  $S$  and  $\Sigma$  are some functions and their typical forms are listed in [1]. Assuming that the tumour boundary is prescribed by a curve  $\Gamma(t, x, y) = 0$ , where  $\Gamma$  is an unknown function, the boundary conditions have the form

$$\begin{aligned} u^1\Gamma_x + u^2\Gamma_y &= -\Gamma_t, \quad p = 0, \\ \left[ (2 + \lambda)u_x^1 + \lambda u_y^2 \right]\Gamma_x + \left[ u_y^1 + u_x^2 \right]\Gamma_y &= 0, \\ \left[ u_y^1 + u_x^2 \right]\Gamma_x + \left[ (2 + \lambda)u_y^2 + \lambda u_x^1 \right]\Gamma_y &= 0. \end{aligned} \quad (2)$$

So, we have the nonlinear boundary value problem (1)-(2) with the unknown moving boundary  $\Gamma(t, x, y) = 0$ .

Using the definition proposed in [2] and assuming  $\Gamma$  to be a closed curve for any  $t \geq 0$ , we examined the Lie symmetry and constructed the exact solutions of the boundary value problem (1)-(2). For instance, the following statement takes place:

*The system of nonlinear PDEs (1) with arbitrary functions  $D$ ,  $S$  and  $\Sigma$  is invariant with respect to the infinite-dimensional Lie algebra generated by the Lie symmetry operators*

$$\begin{aligned} \partial_t, \quad F(t)\partial_p, \quad G_g = g(t)\partial_x + \dot{g}\partial_{u^1}, \quad G_h = h(t)\partial_y + \dot{h}\partial_{u^2} \\ J_f = f(t) \left[ y\partial_x - x\partial_y + (u^2 + \frac{f}{f}y)\partial_{u^1} - (u^1 + \frac{f}{f}x)\partial_{u^2} \right]. \end{aligned}$$

*Here  $F$ ,  $f$ ,  $g$ , and  $h$  are arbitrary smooth functions and the upper dot means differentiation with respect to time.*

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**Physics of Nuclei and Elementary Particles**

**The electroweak phase transition in a spontaneously magnetized vacuum**

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We investigate the electroweak phase transition in the Standard Models with accounting for the spontaneous vacuum magnetization. It is known that for the mass of Higgs boson greater than 75 GeV, the electroweak phase transition is second order. But according to Sakharov's conditions for the formation of the baryon asymmetry of the Universe, it should be strong first order. The spontaneously generated fields are temperature dependent and they have an influence on the phase transition.

Chromomagnetic fields  $B_3$  and  $B_8$  have to be created spontaneously in the gluon sector of QCD at temperature  $T > T_d$  higher than the deconfinement temperature  $T_d$ . Usual magnetic field  $H$  should also be spontaneously generated because of quark-loop. For  $T$  near  $T_{EW}$ , this field should be present too, so they can change the behavior of phase transition.

The critical temperature for the electroweak phase transition is estimated in Standard model and in the scalar theory. The field strengths  $B_3(T)$ ,  $B_8(T)$  and  $H(T)$  at relevant temperatures are also estimated.



**Physics of Nuclei and Elementary Particles**

**Non-congruent phase transitions in strongly interacting matter within the Quantum van der Waals model**

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The non-congruent liquid-gas phase transition (LGPT) in asymmetric nuclear matter is studied using the recently developed Quantum van der Waals model in the grand canonical ensemble. Different values of the electric-to-baryon charge ratio,  $Q/B$ , are considered. This non-congruent LGPT exhibits several features which are not present in the congruent LGPT of symmetric nuclear matter. These include a continuous phase transformation, a change in the location of the critical point, and the separation of the critical point and the endpoints. The effects which are associated with the non-congruent LGPT become negligible for the following cases: when  $Q/B$  approaches its limiting values, 0.5 or 0, or if quantum statistical effects can be neglected. The latter situation is realized when the particle degeneracy attains large values. The skewness and kurtosis of the baryonic and electric charges fluctuations were calculated along the chemical freeze-out curve of nucleus-nucleus collisions within Quantum van der Waals - Hadron Resonance Gas model. Due to the existence of the non-congruent LGPT, all four quantities demonstrate large deviations from the Ideal Hadron Resonance Gas baseline.

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