

# **X Conference of Young Scientists "Problems of Theoretical Physics"**

## **Report of Contributions**

Contribution ID: 1

Type: **Oral**

## The influence of the three-particle interaction on critical phenomena of the Bose-Hubbard Model

*Monday, 23 December 2019 16:25 (20 minutes)*

The critical behavior of a mixture of two types of ultracold bosons on the optical lattice was studied. The system can be described by the Bose-Hubbard model. It is known that the system can be in a superfluid or in a Mott insulator state, depending on the hopping parameter and chemical potential. The interaction between different types of particles drastically changes the phase diagram. In particular, the transitions between mixed and superfluid states appear. The presence of a three-particle interaction leads to an increase in the Mott insulator region of the phase diagram. In particular, bosons with a higher hopping value can be still in the Mott insulator phase. The results are obtained in the framework of the mean-field approximation for a wide range of parameters.

**Primary authors:** Mr KRYVCHIKOV, Oleksii (B.Verkin Institute for Low Temperature Physics and Engineering of the National Academy of Sciences of Ukraine); Prof. ZALESSKI, Tomasz (Instytut Niskich Temperatur i Badań Strukturalnych PAN)

**Presenter:** Mr KRYVCHIKOV, Oleksii (B.Verkin Institute for Low Temperature Physics and Engineering of the National Academy of Sciences of Ukraine)

**Session Classification:** Statistical Theory of Many-body Systems

**Track Classification:** Statistical Theory of Many-body Systems

Contribution ID: 3

Type: **Oral**

## Dark-matter admixed compact stars and their properties under extreme conditions

*Tuesday, 24 December 2019 11:35 (20 minutes)*

We study an impact of asymmetric dark matter on properties of the neutron stars and their ability to reach the two solar masses limit, which allows us to present a new upper constraint on the mass of dark matter particle. Our analysis is based on the observational fact of existence of three pulsars reaching this limit and on the theoretically predicted reduction of the neutron star maximal mass caused by accumulation of dark matter in its interior. Using modern data on spatial distribution of baryon and dark matter in the Milky Way we argue that particles of dark matter can not be heavier than 5 GeV. We also demonstrate that light dark matter particles with masses below 0.2 GeV can create an extended halo around the neutron star leading not to decrease, but to increase of its visible gravitational mass. Furthermore, we predict that high precision measurements of the neutron stars maximal mass near the Galactic center will put a stringent constraint on the mass of the dark matter particle. This last result is particularly important to prepare ongoing, and future radio and X-ray surveys.

**Primary authors:** Dr SAGUN, Violetta (University of Coimbra, Portugal/ Bogolyubov Institute for Theoretical Physics National Academy of Sciences of Ukraine, Kyiv); Dr IVANYTSKYI, Oleksii (Bogolyubov Institute for Theoretical Physics National Academy of Sciences of Ukraine, Kyiv); Prof. LOPES, Ilidio ( University of Coimbra, Portugal)

**Presenter:** Dr SAGUN, Violetta (University of Coimbra, Portugal/ Bogolyubov Institute for Theoretical Physics National Academy of Sciences of Ukraine, Kyiv)

**Session Classification:** Astrophysics and Cosmology

**Track Classification:** Astrophysics and Cosmology

Contribution ID: 4

Type: **Oral**

## Thermal counterflow and electrical activity of superfluid systems in a magnetic field

*Monday, 23 December 2019 10:15 (20 minutes)*

It is shown that the thermal counterflow in superfluid helium placed in a magnetic field leads to the appearance of an electric field in the surrounding space. The effect is due to the counterflow nature of thermal conductivity in superfluid systems: heat transfer in such systems is associated with the movement of the normal component, but the average mass flow carried by the normal component is compensated by the mass flow carried by the superfluid component. The local mass flow is nonzero. The effect occurs for stationary and non-stationary (second sound) heat flow. The features of the effect for samples with different geometries are considered. It was established that the magnitude of the arising electric field substantially depends on the shape of the sample and the direction of the magnetic field [1].

[1] S.I. Shevchenko, A.M. Konstantinov, JETP Lett. 109, 790-794, (2019).

**Primary authors:** Mr KONSTANTINOV, Aleksandr (B.Verkin Institute for Low Temperature Physics and Engineering of the National Academy of Sciences of Ukraine); Dr SHEVCHENKO, Sergey (B.Verkin Institute for Low Temperature Physics and Engineering of the National Academy of Sciences of Ukraine)

**Presenter:** Mr KONSTANTINOV, Aleksandr (B.Verkin Institute for Low Temperature Physics and Engineering of the National Academy of Sciences of Ukraine)

**Session Classification:** Condensed Matter Physics

**Track Classification:** Condensed Matter Physics

Contribution ID: 5

Type: **Poster**

## Compressibility excess and structurization of binary granular mixture

*Monday, 23 December 2019 17:30 (5 minutes)*

We consider the property of compressibility of the binary granular mixture paying attention to their local structurization. The Kirkwood-Buff theory [1] has been used in order to provide theoretical description of the free volume and compressibility of model bi-component system [2]. Relevant characters of compactivity has been expressed in terms of partial properties of species. For theoretical modelling of respective reference data we use either hard sphere model or phenomenological data extracted from the physical measurement [3,4].

We show the existence of the nonmonotonic character of the velocity of compaction (different time-scale kinetics) and polodispersive content of system which pass the compression.

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[4]. Pilliteri S., Lumay G., Opsomer E., Vandewalle N. From jamming to fast compaction dynamics in granular binary mixtures. Sci. Rep. 9, 7281 (2019); <https://doi.org/10.1038/s41598-019-43519-6>

**Primary author:** SIDLETSKA, Liudmyla (Odesa State Environmental University)

**Co-authors:** Mr SPIVAK, Andrii (Odesa State Environmental University); Prof. GERASYMOV, Oleg (Odesa State Environmental University)

**Presenter:** SIDLETSKA, Liudmyla (Odesa State Environmental University)

**Session Classification:** Poster session

**Track Classification:** Statistical Theory of Many-body Systems

Contribution ID: 6

Type: **Poster**

## Symmetry breaking in weak- and strong- coupled ring-shaped superflows of Bose–Einstein condensates

*Monday, 23 December 2019 17:35 (5 minutes)*

One of the most remarkable manifestations of quantum properties of superconductors and superfluids is formation of Josephson vortices (JVs), alias fluxons, in long Josephson junctions.

In this work, we studied weak- and strong-coupled systems of two parallel superfluid rings with different angular momenta. Atomic Bose-Einstein condensates loaded in a dual-ring trap (two rings separated by a horizontal potential barrier) suggest a possibility to consider the tunneling dynamics.

Our research corresponds with investigation of tunneling influence on dynamics of coupled ring-shaped systems of superflows by numerical simulations in framework of weakly dissipative mean-field model.

In case of weak-coupling, symmetry breaking suggests Josephson vortex nucleation between the superflows with different angular momenta in low density area.

In case of strong-coupling (when the barrier is gradually eliminated), we observed the following situation: the JVs accumulate more and more energy and there is substantially 3D dynamics of vortices. We describe dynamics of counter-rotating superflows with and without axial symmetry breaking. It is demonstrated that the population imbalance between the merging flows and the breaking of the underlying rotational symmetry can drive the double-ring system to final states with different angular momenta.

**Primary authors:** Dr YAKIMENKO, Alexander (Department of Physics, Taras Shevchenko National University of Kyiv); Dr MALOMED, Boris (Department of Physical Electronics, Faculty of Engineering, and Center for Light-Matter Interaction, Tel Aviv University); Mr YATSUTA, Igor (Department of Physics, Taras Shevchenko National University of Kyiv); Mr OLIINYK, Artem (Department of Physics, Taras Shevchenko National University of Kyiv)

**Presenter:** Mr OLIINYK, Artem (Department of Physics, Taras Shevchenko National University of Kyiv)

**Session Classification:** Poster session

**Track Classification:** Condensed Matter Physics

Contribution ID: 7

Type: **Oral**

## Towards understanding of condensed matter via study granular systems

Monday, 23 December 2019 16:45 (20 minutes)

Granular materials under the external perturbations show a diversity of structural transformations which characterized by different symmetries. Their rigorous classification in terms of phase transitions seems very attractable (nevertheless, still questionable). Intriguing question is: can we use the information extracted from studying of structural transformations characters in granular materials to describe any details about the local symmetry of the condensed matter, which displayed during the typical phase-transformations? Here, there are several analogies as well as discrepancies are waiting for us: Local structure, Phase transitions, Landau-Ginzburg kinetics, Lindeman criteria for crystallization, Equation of state.

We would like to outline some results of our research directed to study of structurization, which occurs during packing processes in gently agitated granular (micro-mechanical) systems [1-5]. The focus will be done on developing and investigation of hard-spheres (discs) packing models. The results of this research, in our opinion, in principle can provide an understanding of some characters of the local structure and bulk properties not only of granular matter, but also a regular phases of condensed matter (e.g., molecular liquids and solutions, colloids, glasses). The problem of densest packing are formally belong to pure mathematical area. But inspite of this objectives to study structural and physical properties of perturbed granular systems a variety of physical theoretical models which are partially based on phenomenological information (direct observation) have been developed. The packing of hard-particles can be described by geometric approach, which provides a practical and universal methods of quantitative characterization of the local (as well as global) packing via symmetry categories.

We will consider a packing of a large conglomeration of hard particles confined by a finite-sized container. Boundaries as well as exclusion-volume effects (under the negligible dissipation) would be described by simple packing parameters (like compactivity). Properties of the states of such systems (for instance 2D hard discs) will be studied theoretically and after then compared with the results of direct observations. Obtained results will be analyzed with respect to reminiscences with some properties of the typical phases of condensed matter.

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- [5]. Schockmel J., Vandewalle N., Opsomer E., Lumay G. Frustrated crystallization of a monolayer of magnetized beads under geometrical confinement. *Phys. Rev. E* 95 (6), 062120 (2017). DOI: <https://doi.org/10.1103/PhysRevE.95.062120>

**Primary author:** Mr SPIVAK, Andrii (Odesa State Environmental University)

**Co-author:** Prof. GERASYMOV, Oleg (Odesa State Environmental University)

**Presenter:** Mr SPIVAK, Andrii (Odesa State Environmental University)

**Session Classification:** Statistical Theory of Many-body Systems

**Track Classification:** Statistical Theory of Many-body Systems

Contribution ID: 8

Type: **Poster**

## Ferroelectric nanocomposites: influence of nanoparticle sizes distribution on pyroelectric and electrocaloric conversion parameters

*Monday, 23 December 2019 17:45 (5 minutes)*

Pyroelectric (PE) and electrocaloric (EC) properties on the ferroelectric-antiferroelectric phase boundary of ferroelectric (FE) thin films, multilayers and other low-dimensional materials can significantly differ from PE and EC properties of bulk single crystals, solid solutions and ceramics. In fact, even for FE nanoparticles, for which efficient synthesis procedures and methods for controlling polar properties have already been developed, there are still many technological problems [1] and the mysteries of theory [2]. In particular, under consideration of EC effect in BaTiO<sub>3</sub> nanoparticle within the core-shell model [3], the depolarization effects, which are inevitable in the case of zero polarization, were completely neglected. This fact does not allow to apply the obtained in Ref. [1] results to real systems. Using phenomenological Landau-Ginsburg-Devonshire theory and the approximation of the effective medium, typical dependences of the parameters PE and EC conversion on the external electric field, temperature, and radius for spherical monodomain FE nanoparticles with fixed radius were calculated analytically in Ref. [4]. In this work typical dependences of the parameters PE and EC conversion for nanocomposites with spherical monodomain FE nanoparticles of different sizes have been calculated analytically.

[1]. U. Idehenre, Y. A. Barnakov, S. A. Basun, D. R. Evans, Spectroscopic studies of the effects of mechanochemical synthesis on BaTiO<sub>3</sub> nanocolloids prepared using high-energy ball-milling, *J. Appl. Phys.*, 124, pp. 165501-1-5, (2018).

[2]. Y. A. Barnakov, I. U. Idehenre, S. A. Basun, T. A. Tyson, D. R. Evans, Uncovering the mystery of ferroelectricity in zero dimensional nanoparticles, *Nanoscale Advances*, 1, pp. 664-670, (2019).

[3]. C. Xiqu and C. Fang, Study of electrocaloric effect in barium titanate nanoparticle with core-shell model, *Physica B: Cond. Matt.*, 415, pp. 14-17 (2013).

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**Primary author:** Ms SHEVLIKOVA, Hanna (Department of Microelectronics, National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", Kyiv, Ukraine)

**Presenter:** Ms SHEVLIKOVA, Hanna (Department of Microelectronics, National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", Kyiv, Ukraine)

**Session Classification:** Poster session

**Track Classification:** Condensed Matter Physics

Contribution ID: 9

Type: Oral

## Localized waves and resonance effects in layered superconductors

Monday, 23 December 2019 10:55 (20 minutes)

High-temperature superconductors with layered structure, such as  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ ,  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ ,  $\text{La}_{2-\delta}\text{Sr}_\delta\text{CuO}_4$  are anisotropic and strongly nonlinear Josephson plasma media. Such layered superconductors favor propagation of electromagnetic waves in the THz frequency range which is promising for various applications. In close analogy to nonlinear optics, these materials exhibit numerous remarkable features, including the self-focusing effects, slowing down of light, stimulated transparency etc. Furthermore, layered superconductors possess anisotropy with simultaneously different signs of the permittivity tensor components in a certain frequency range, providing a possibility of negative index of refraction and hyperbolic dispersion law [1].

In this work, a series of recent theoretical studies of the propagation of localized Josephson plasma waves (JPW) in layered superconductors is discussed. In particular, the propagation of JPWs along the boundaries of semi-infinite samples and along a plate of finite thickness are studied. We show that when the layers are perpendicular to the plate boundaries, the anomalous dispersion of the localized waves is predicted for layered superconductors in a certain range of frequencies and wave numbers [2]. In addition, due to nonlinearity one can control the anomalous dispersion of the spectrum by the wave amplitude [3].

We also present new results on excitation and propagation of localized Josephson plasma waves in a plate of layered superconductor in the presence of an external static magnetic field. For this case, the dispersion equations for localized waves in the plate of layered superconductor are obtained. It turns out that even relatively weak static magnetic field can significantly change the conditions for the waves propagation [4]. Also, we study THz transmission through layers and show that the resonance transmission of JPWs can be flexibly tuned by the DC magnetic field in a wide range of the parameters. The studied resonant phenomenon opens wide prospects for possible applications, such as THz waves filtering or tuning the emission and receive frequency from THz sources.

The publication contains the results of studies conducted by Presidents of Ukraine grant for competitive projects (F82/233-2019), which support we gratefully acknowledge.

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[2]. S.S. Apostolov, Z.A. Maizelis, D.V. Shimkiv, A.A. Shmat'ko, V.A. Yampol'skii, Low Temp. Phys. 45, 885 (2019).

[3]. S.S. Apostolov, D.V. Kadygrob, Z.A. Maizelis, A.A. Nikolaenko, V.A. Yampol'skii, Low Temp. Phys. 44(3), 238 (2018).

[4]. T. Rokhmanova, S.S. Apostolov, N. Kvitka, V.A. Yampol'skii, Low Temp. Phys. 44, 552 (2018).

**Primary authors:** Dr KADYGROB, Dmytro (A.Ya. Usikov Institute for Radiophysics and Electronics National Academy of Sciences of Ukraine, Kharkov, Ukraine\ V.N. Karazin Kharkov National University, Kharkov, Ukraine); Dr ROKHMANOVA, Tetiana (Universidad de Murcia, Departamento de Fisica - CIOyN, Murcia, Spain\ A.Ya. Usikov Institute for Radiophysics and Electronics National Academy of Sciences of Ukraine, Kharkov, Ukraine); Dr APOSTOLOV, Stanislav (A.Ya. Usikov Institute for Radiophysics and Electronics National Academy of Sciences of Ukraine, Kharkov, Ukraine\ V.N. Karazin Kharkov National University, Kharkov, Ukraine); Prof. YAMPOL'SKII, Valeriy (A.Ya. Usikov Institute for Radiophysics and Electronics National Academy of Sciences of Ukraine, Kharkov, Ukraine\ V.N.

Karazin Kharkov National University, Kharkov, Ukraine)

**Presenter:** Dr KADYGROB, Dmytro (A.Ya. Usikov Institute for Radiophysics and Electronics National Academy of Sciences of Ukraine, Kharkov, Ukraine\ V.N. Karazin Kharkov National University, Kharkov, Ukraine)

**Session Classification:** Condensed Matter Physics

**Track Classification:** Condensed Matter Physics

Contribution ID: 10

Type: **Oral**

## On fast charged particles scattering in thin crystalline and amorphous targets

*Tuesday, 24 December 2019 16:15 (20 minutes)*

The problem of fast charged particles scattering in a thin layer of crystalline and amorphous matter is considered [1]. There is suggested an approach that allows one to consider the process of scattering in such targets from a single point of view. The approach is based on the Born and Eikonal approximations of the quantum scattering theory [2]. In the case of scattering in a crystal, special attention is paid to the question of the cross section splitting into coherent and incoherent components and to the applicability conditions of the Born and Eikonal approximations for different orientations of the crystal axes and planes.

### References

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- [2] A.I. Akhiezer, N.F. Shul'ga. High Energy Electrodynamics in Matter. Gordon and Breach Pub. Amsterdam. 1996

**Primary authors:** Dr SHUL'GA, Nikolai (National Science Center Kharkiv Institute of Physics and Technology, Kharkiv); KORIUKINA, Viktoriia (National Science Center Kharkiv Institute of Physics and Technology, Kharkiv)

**Presenter:** KORIUKINA, Viktoriia (National Science Center Kharkiv Institute of Physics and Technology, Kharkiv)

**Session Classification:** Physics of Nuclei and Elementary Particles

**Track Classification:** Physics of Nuclei and Elementary Particles

Contribution ID: 11

Type: Oral

## Dark matter signals description in the scattering processes in the generalized Yukawa model

Tuesday, 24 December 2019 15:15 (20 minutes)

According to present day results of the LHC experiment data analysis, there were no dark matter candidates found. The purpose of this work is to present a possible theoretical explanation why it could be so.

In our consideration, we propose a simple dark matter model of the heavy fermions described by the field  $\psi$ . A visible matter is modeled by the pair of scalar fields – light  $\phi$  and heavy  $\chi$ . These fields interact with dark matter through Yukawa's couplings. Besides, there is the doublet of fermions fields  $\psi_1$  and  $\psi_2$  interacting with  $\phi$  and  $\chi$  with different couplings. The Yukawa model is chosen as the simplest one for the interaction carrier, which allows us to take into consideration the qualitatively important effect of the coupling constant values. At the same time, the transformation properties of visible fields are not accounted for as inessential.

We start from the Lagrangian:

$$\mathcal{L} = \frac{1}{2} [(\partial_\nu \phi)^2 - \mu^2 \phi^2] + \frac{1}{2} [(\partial_\nu \chi)^2 - \Lambda^2 \chi^2] + \quad (1)$$

$$+ \sum_{a=1;2} \bar{\psi}_a (i\gamma^\nu \partial_\nu - g_\phi \phi - g_\chi \chi - m) \psi_a + \bar{\Psi} (i\gamma^\nu \partial_\nu - M) \Psi - \quad (2)$$

$$- \lambda \phi^4 + \rho \phi^2 \chi^2 - \xi \chi^4 - G_\chi \bar{\Psi} \chi \Psi. \quad (3)$$

As we see, fermions interact with each other via the interchange of scalar particles. It can be considered as the effective four-fermions vertexes. Probability of certain scenario of interaction – through  $\phi$  or  $\chi$  field – depends on the mixing angle between these two fields. Moreover, the polarization tensor of  $\chi$  contains also the contribution of the  $\Psi$  fermion loop. Hence, the differential cross-section  $\sigma$  of the four-fermions interaction depends on the mass of the dark matter particle and the mixing angle between scalar fields. We set this angle to be equalled  $10^{-3}$ - $10^{-4}$ , while the mass of  $\Psi$  is much bigger than the mass of  $\psi_1$  or  $\psi_2$ . Because of this, a cross-section width becomes significant, so that such a signal can be missed in the data analysis on the LHC as a noise. This is probably because the narrow width approximation is applied in processing of data treating applied by Collaborations. Taking into account the facts listed above, the differential cross-section of the four-fermion interaction is obtained and its spatial angular dependence is investigated. The renormalisations of the couplings and masses are fulfilled. We investigate how the  $\sigma$  changes dependently on the  $\Psi$  field mass and the mixing angle of scalar fields. Process  $\bar{\psi}_1 \psi_1 \rightarrow \bar{\psi}_2 \psi_2$  is considered.

A. Gulov, A. Kozhushko, V. Skalozub. Global search for the  $Z'$  boson in scattering processes - Дніпро: ЛІРА, 2018. - 124 с.

**Primary authors:** Mr DMYTRIIEV, Mykyta (Oles Honchar Dnipro National University); SKALOZUB, Vladimir (Oles Honchar Dnipro National University)

**Presenter:** Mr DMYTRIIEV, Mykyta (Oles Honchar Dnipro National University)

**Session Classification:** Physics of Nuclei and Elementary Particles

**Track Classification:** Physics of Nuclei and Elementary Particles

Contribution ID: 12

Type: **Oral**

## Chern-Simons portal

*Tuesday, 24 December 2019 17:55 (20 minutes)*

The Standard Model (SM) is the best theory of particle physics for today, giving precise predictions. However, it fails to explain some fundamental problems such as the strong CP problem, neutrino oscillations, matter-antimatter asymmetry, and the nature of dark matter and dark energy.

To resolve these problems it seems reasonable to add new particles to the SM. Since these particles are not detected they can be either very heavy (with a mass more than energy scale of the available accelerators) or light but very weakly interacting with the SM particles. The particles of the last type, also called feebly interacting massive particles (FIMPs), can be searched in intensity frontier experiments like SHiP.

One can classify FIMPs by their type: scalar, pseudoscalar, fermion, vector or pseudovector particles and interaction with SM. The most promising to search are such interactions that connect FIMP to the SM in a renormalizable way or using low-order operators. If these particles are light their parameters and interaction with the SM particles can be determined by physics at a very large scale.

In this talk, we considered the Chern-Simons extension of the SM by the new light pseudovector particle because this extension of the SM was relatively recently proposed and it is not sufficiently studied.

We have analytically calculated the process of heavy quark decay into light quark and pseudovector boson that allows us to calculate the process of heavy meson decay with Chern-Simons particle production. These results will be used to find the sensitivity of the SHiP experiment to detect Chern-Simons particles.

**Primary authors:** GORKAVENKO, Volodymyr (Taras Shevchenko National University of Kyiv, Faculty of Physics); Mr KASHKO, Pavlo (Taras Shevchenko National University of Kyiv, Faculty of Physics); Mr BONDARENKO, Kyrylo (Theoretical Physics Department, CERN, 1 Esplanade des Particules, Geneva 23, CH-1211, Switzerland)

**Presenter:** Mr KASHKO, Pavlo (Taras Shevchenko National University of Kyiv, Faculty of Physics)

**Session Classification:** Physics of Nuclei and Elementary Particles

**Track Classification:** Physics of Nuclei and Elementary Particles

Contribution ID: 13

Type: **Lecture**

## **Hunting the dark matter origin with astrophysical and cosmological data**

*Tuesday, 24 December 2019 09:30 (45 minutes)*

**Primary author:** Dr IAKUBOVSKYI, Dmytro (Bogolyubov Institute for Theoretical Physics)

**Presenter:** Dr IAKUBOVSKYI, Dmytro (Bogolyubov Institute for Theoretical Physics)

**Session Classification:** Astrophysics and Cosmology

**Track Classification:** Astrophysics and Cosmology

Contribution ID: 14

Type: **Oral**

## The electroweak phase transition and spontaneous creation of magnetic fields

*Tuesday, 24 December 2019 14:55 (20 minutes)*

There were many phase transitions during the evolution of our Universe. The electroweak phase transition and deconfinement were two of them. The electroweak phase transition happened near 100 GeV and due to Higgs mechanism the leptons, quarks and gauge bosons gained mass. The deconfinement phase transition happened near 150 MeV and quarks combined to each other, as a result baryons and mesons were created. In QCD and gluodynamics the color chromomagnetic fields  $B_3$  and  $B_8$  are created spontaneously at temperature  $T > T_d$  higher than the deconfinement temperature  $T_d$ . Usual magnetic field  $H$  had also been spontaneously generated because of quarks loop. The quarks possess electric and color charges, as a result magnetic and chromomagnetic fields are mixing in effective potential. These fields appear spontaneously for  $T > T_d$  and they were present for temperature near critical temperature of the electroweak phase transition. For  $T$  close to  $T_{EW}$  the magnetic fields could change the type of the phase transition.

We investigate the electroweak phase transition in the Standard Model with accounting the spontaneously generated magnetic and chromomagnetic fields. As it is known, for the mass of Higgs boson greater than 75 GeV this phase transition is second order. But according to Sakharov's conditions for the formation of the baryon asymmetry of the Universe it has to be strongly first order. The spontaneously generated (chromo) magnetic fields are temperature dependent. They influence the phase transition. The strength of generated fields and the critical temperature of phase transition are also estimated.

**Primary authors:** Mr MINAIEV, Pavlo (Oles Honchar Dnipro National University); Prof. SKALOZUB, Vladimir (Oles Honchar Dnipro National University)

**Presenter:** Mr MINAIEV, Pavlo (Oles Honchar Dnipro National University)

**Session Classification:** Physics of Nuclei and Elementary Particles

**Track Classification:** Physics of Nuclei and Elementary Particles

Contribution ID: 15

Type: Oral

# The verification of Machine Learning methods for binary morphological classification of SDSS-galaxies

Tuesday, 24 December 2019 10:55 (20 minutes)

Classification of galaxy types is one of the cornerstones for extragalactic astrophysics and observational cosmology. The most precise method of galaxy classification used by astronomers so far is the manual classification. Its major drawback, however, is the extensive usage of manpower, either from highly skilled professionals, or, in some cases (such as in Galaxy Zoo project) amateur astronomers. Modern or forthcoming galaxy surveys (SDSS, LSST, DES, KiDS, etc.) are able to detect hundreds of millions of galaxies, impossible to classify manually. This exaggerates the interest to use the alternatives in form of various recently developed Machine Learning (including Deep Learning) techniques for automated classification of galaxies.

We present a study on the verification of Machine Learning (ML) methods to be applied for binary morphological classification of galaxies (*E* - Early and *L* - Late types). We used two kinds of supervised learning techniques: the first is classical machine learning classifiers, and the second is deep convolutional neural network classifier.

We want to emphasize that, unlike most other authors, we paid attention to the visual cleaning of the dataset. Our dataset contains of  $\sim 300\,000$  SDSS-galaxies from DR9 with unknown morphological types at  $z < 0.1$  redshift. The training galaxy sample contains of  $\sim 6\,000$  galaxies with the visually inspected morphological types selected randomly with different redshifts and luminosity from the total sample.

We applied the following classical machine learning classifiers: Naive Bayes, Random Forest, Support Vector Machines, Logistic Regression, and k-Nearest Neighbor algorithm. To study the classifier, we used absolute magnitudes, color indices and inverse concentration index to the center. It turned out that Support Vector Machine Classifiers provide a highest accuracy - 96.4 % (96.1 % - *E* and 96.9 % - *L*).

We used the deep convolutional neural network classifier, namely Xception, to provide a classification of (g-r-i) composite images (25 arcsec in each axis in size) of SDSS-galaxies. We provided the data augmentation (horizontal and vertical flips, random shifts on  $\pm 10$  pixels, and rotations within 180 degrees), that was randomly applied to the images during learning. It turned out that deep convolutional neural network provide accuracy - 93.5 % (95 % - *E* and 86 % - *L*).

We compared our results and proposed a method to learn the benefits from both approaches (classical machine learning classifiers and deep convolutional neural network classifier). We show the common mistakes of both algorithms, and propose to stack these two approaches to block these mistakes, with a main goal to increase the overall classification quality of SDSS galaxies.

**Primary authors:** Dr DOBRYCHEVA, Daria (Main Astronomical Observatory of the National Academy of Sciences of Ukraine); Mr VASYLENKO, Maksym (Main Astronomical Observatory of the National Academy of Sciences of Ukraine); Mr KHRAMTSOV, Vlad (Institute of Astronomy, V.N. Karazin Kharkiv National University); Dr VAVILOVA, Irina (Main Astronomical Observatory of the National Academy of Sciences of Ukraine)

**Presenter:** Dr DOBRYCHEVA, Daria (Main Astronomical Observatory of the National Academy of Sciences of Ukraine)

**Session Classification:** Astrophysics and Cosmology

**Track Classification:** Astrophysics and Cosmology

Contribution ID: 16

Type: **Oral**

## New mass bound on fermionic dark matter from a combined analysis of classical dSphs

*Tuesday, 24 December 2019 10:15 (20 minutes)*

Dwarf spheroidal galaxies (dSphs) are the most compact dark-matter-dominated objects observed so far. The Pauli exclusion principle limits the number of fermionic dark matter particles that can compose a dSph halo. This results in a well-known lower bound on their particle mass. So far, such bounds were obtained from the analysis of individual dSphs. We model dark matter halo density profiles via the semi-analytical approach and analyse for the first time the data from eight ‘classical’ dSphs assuming the same mass of dark matter fermion in each object. We obtain a new  $2\sigma$  lower bound of  $m \gtrsim 190$  eV on the dark matter fermion mass. Besides, by combining a sub-sample of four dSphs – Draco, Fornax, Leo I, and Sculptor – we conclude that 220 eV fermionic dark matter appears to be preferred over the standard cold dark matter at about  $2\sigma$  level. However, this result becomes insignificant if all seven objects are included in the analysis.

**Primary author:** SAVCHENKO, Denys (Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Kyiv)

**Co-author:** RUDAKOVSKYI, Anton (Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Kyiv)

**Presenter:** SAVCHENKO, Denys (Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Kyiv)

**Session Classification:** Astrophysics and Cosmology

**Track Classification:** Astrophysics and Cosmology

Contribution ID: 17

Type: **Poster**

## New bounds on axion-like particles from NuSTAR observations

*Monday, 23 December 2019 18:10 (5 minutes)*

Axions are hypothetical particles beyond the Standard Model. Their existence is postulated to resolve the strong CP problem in QCD. The existence of the axion-like particles should modify the visible spectra of the cosmic objects due to their coupling to photons in the presence of a magnetic field, for example, inside galaxy clusters. For this reason, they were proposed as one of the explanations for the inconsistencies between Hitomi and Chandra observations of the 3.5 keV line in Perseus cluster. Furthermore, axion-like particles could constitute the cold dark matter itself.

In this talk, we present the upper bounds on the axion-photon coupling from non-detection of imprints of such coupling in the NuSTAR observations of the NGC1275 galaxy, embedded in the Perseus galaxy cluster.

**Primary author:** SAVCHENKO, Denys (Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Kyiv)

**Co-author:** Dr MALYSHEV, Denys (Eberhard Karls Universität Tübingen)

**Presenter:** SAVCHENKO, Denys (Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Kyiv)

**Session Classification:** Poster session

**Track Classification:** Astrophysics and Cosmology

Contribution ID: 18

Type: **Oral**

## Static and slowly rotating three-dimensional black hole in nonlinear electrodynamics

*Tuesday, 24 December 2019 12:15 (20 minutes)*

Three-dimensional electrically charged black hole with nonlinear electromagnetic field in anti-de Sitter spacetime is studied. Both static [1] and slowly rotating cases are considered. Solutions of field equations are obtained and thermodynamic behavior in extended phase space thermodynamics is examined.

[1] M. B. Tataryn, M. M. Stetsko, *Int. J. Mod. Phys. D* 28 (2019) 1950160.

**Primary authors:** Mr TATARYN, Mykhailo (Department for Theoretical Physics, Ivan Franko National University of Lviv); Mr STETSKO, Mykola (Department for Theoretical Physics, Ivan Franko National University of Lviv)

**Presenter:** Mr TATARYN, Mykhailo (Department for Theoretical Physics, Ivan Franko National University of Lviv)

**Session Classification:** Astrophysics and Cosmology

**Track Classification:** Astrophysics and Cosmology

Contribution ID: 19

Type: **Poster**

## Analogue Hawking radiation in a ring of Bose-Einstein condensate

*Monday, 23 December 2019 17:40 (5 minutes)*

Hawking radiation is one of the most fascinating phenomena taking place near the black hole horizon. Featuring both gravitational and quantum properties this effect is extremely hard to observe on the real objects. Surprisingly, it is possible to mimic evaporation of particles on the acoustic analogs, where Bose-Einstein condensate plays a role of background giving birth for Hawking pairs. This area is still a matter of multiple discoveries providing us with the very first convincing observation of Hawking effect analog this year.

We address a model of effectively one-dimensional (1D) Bose-Einstein condensate (BEC) confined in a toroidal trap. This system is attractive to explore since the total flow of quantum liquid is quantized which results in a restriction on possible values of the velocity of the condensate. Moreover, it is impossible to avoid the presence of the so-called white hole (inner) horizon in such toroidal geometry.

Unlike recent works on the acoustic horizon in toroidal BECs, we apply the method previously used for modeling an infinitely long quasi-one-dimensional condensate to our system. It allows to create acoustic horizons in the condensate with uniform density. Remarkably, we managed to see the correlation pattern having the properties of the analog Hawking effect. Obtained correlations turned out to be strongly dependent on the length of the ring and initial noise for the fixed parameters of the horizon. Furthermore, for some particular size of the region Hawking correlations disappear that may be an interesting analogy of the existence of Planck mass limit for real black holes. Also, we considered the influence of the white hole horizon on the correlation pattern and stability of the system for different values of surface gravity.

**Primary authors:** YATSUTA, Igor (Department of Physics, Taras Shevchenko National University of Kyiv); Dr YAKIMENKO, Alexander (Department of Physics, Taras Shevchenko National University of Kyiv)

**Presenter:** YATSUTA, Igor (Department of Physics, Taras Shevchenko National University of Kyiv)

**Session Classification:** Poster session

**Track Classification:** Condensed Matter Physics

Contribution ID: 20

Type: **Oral**

## Equation of state from lattice QCD at imaginary chemical potential and external magnetic field

*Tuesday, 24 December 2019 14:35 (20 minutes)*

This report is devoted to lattice study of QCD equation of state (EOS) at finite baryon chemical potential and nonzero magnetic field. The simulations are performed with rooted dynamical staggered  $u$ ,  $d$ ,  $s$  quarks at physical quark masses. In order to avoid the sign problem, the study is carried out at imaginary chemical potential and the results are analytically continued to real chemical potential. In this report we present our preliminary results for the pressure and energy density for various values of temperature, chemical potential and magnetic field.

**Primary authors:** Dr NIKOLAEV, Aleksandr (Department of Physics, College of Science, Swansea University, United Kingdom); Dr KOTOV, Andrey (Joint Institute for Nuclear Research, Dubna, Russia); Ms KOLOMOYETS, Natalia (Joint Institute for Nuclear Research, Dubna, Russia); Dr ASTRAKHANTSEV, Nikita (Universitat Zurich, Switzerland); Dr BRAGUTA, Victor (Joint Institute for Nuclear Research, Dubna, Russia)

**Presenter:** Ms KOLOMOYETS, Natalia (Joint Institute for Nuclear Research, Dubna, Russia)

**Session Classification:** Physics of Nuclei and Elementary Particles

**Track Classification:** Physics of Nuclei and Elementary Particles

Contribution ID: 21

Type: **Oral**

## Second look to the Polyakov Loop Nambu-Jona-Lasinio model at finite baryonic density

*Tuesday, 24 December 2019 14:15 (20 minutes)*

We revisit the Polyakov Loop coupled Nambu-Jona-Lasinio model that maintains the Polyakov loop dynamics in the limit of zero temperature, which is of interest for astrophysical applications. For this purpose we re-examine the form of the potential for the deconfinement order parameter at finite baryonic densities. Secondly, and the most important, we explicitly demonstrate that a modification of this potential at any temperature is formally equivalent to assigning a baryonic charge to gluons. In order to avoid this spurious effect we develop a more general formulation of the present model that cures this defect and is normalized to match the asymptotic behaviour of the QCD equation of state given by  $\mathcal{O}(\alpha_s^2)$  and partial  $\mathcal{O}(\alpha_s^3 \ln^2 \alpha_s)$  perturbative results.

**Primary authors:** IVANYTSKYI, Oleksii (Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Kyiv); PEREZ-GARCIA, Maria Angeles (University of Salamanca); SAGUN, Violetta (Center for Astrophysics and Gravitation, Instituto Superior Tecnico, Portugal/ Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Kyiv); ALBERTUS, Conrado (University of Salamanca)

**Presenter:** IVANYTSKYI, Oleksii (Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Kyiv)

**Session Classification:** Physics of Nuclei and Elementary Particles

**Track Classification:** Physics of Nuclei and Elementary Particles

Contribution ID: 22

Type: Oral

## Polarization effects of algebraically special Maxwell field in the Kerr space-time

Tuesday, 24 December 2019 12:35 (20 minutes)

For obtaining polarization effects in the Kerr space-time we have used algebraically special approach for Maxwell equations [1].

As a consequence, in Kinnersley tetrad Maxwell field is described only by one extremal component  $\varphi_2$ , and the Maxwell equations have closed-form solution [2]:

$$\varphi_2 = C \frac{e^{i\omega(t-\tilde{r})+im\phi}}{\sin\theta(r-ia\cos\theta)} e^{-a\omega\cos\theta} \left(\frac{1-\cos\theta}{\sin\theta}\right)^m,$$

where  $t > 0$ ,  $r_+ < r < \infty$ ,  $0 < \theta < \pi$ ,  $0 \leq \phi < 2\pi$ ,  $\tilde{r} = r + M \ln \Delta + \frac{M^2}{\sqrt{M^2-a^2}} \ln \left(\frac{r-r_+}{r-r_-}\right) + \frac{am}{2\omega\sqrt{M^2-a^2}} \ln \left(\frac{r-r_+}{r-r_-}\right)$ ,  $\omega \in \mathbb{R}$  is a frequency of the wave,  $m \in \mathbb{Z}$  is an azimuthal number,  $M$  is a mass of gravitating body,  $a$  is an angular momentum per unit mass ( $a < M$ ),  $\Delta = r^2 - 2Mr + a^2$ ,  $r_+ = M + \sqrt{M^2 - a^2}$ ,  $r_- = M - \sqrt{M^2 - a^2}$ ,  $C = C_m(\omega)$  is a complex constant.

From the above solution for outgoing waves, we have obtained formulas for Stokes parameters, ellipticity angle and polarization angle, and gravitational analog of Faraday effect. There are distinguished two polarization effects in Kerr field. The first one is the rotation of the plane of polarization (RPP), and the second is the influence of angular momentum of rotating body on an amplitude of right or left circularly polarized waves, discovered for low and high frequencies in [3,4]. Obtained in our approach results confirm the formula of Gnedin and Dymnikova [5] for the RPP, dispersion of the RPP is absent. The influence of angular momentum on amplitude is established by a closed-form expression in the full range of frequencies.

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- [1]. Penrose R., Rindler W. Spinors and space-time. Two-spinor calculus and relativistic fields. Cambridge University Press, 1984, Vol. 1.
- [2]. Pelykh V. O., Taistra Y. V. Ukr. Journ. of Phys. **62**, № 11, 1007 (2017).
- [3]. Barbieri A., Guadagnini E. Nucl. Phys. B **703**, 391-399 (2004).
- [4]. Leite L., Dolan S., Crispino L. arXiv:1707.01144v1 [gr-qc], 4 Jul 2017.
- [5]. Gnedin N. I., Dymnikova I. G. Zhur. Eksp. i Teor. Fiz. **94**, №1, 26 (1988).

**Primary authors:** Mr TAISTRA, Yurii (Pidstryhach Institute for Applied Problems of Mechanics and Mathematics National Academy of Sciences of Ukraine, Lviv); Dr PELYKH, Volodymyr (Pidstryhach Institute for Applied Problems of Mechanics and Mathematics National Academy of Sciences of Ukraine, Lviv)

**Presenter:** Mr TAISTRA, Yurii (Pidstryhach Institute for Applied Problems of Mechanics and Mathematics National Academy of Sciences of Ukraine, Lviv)

**Session Classification:** Astrophysics and Cosmology

**Track Classification:** Astrophysics and Cosmology

Contribution ID: 23

Type: **Oral**

## **Influence of the cell wall on cyanide destruction by bacteria in the model of respiratory mechanism**

*Monday, 23 December 2019 15:25 (20 minutes)*

The research is based on the ideology that the destructive centers of cyanides in living microorganisms are respiratory centers, the destruction of cyanides is investigated. The phenomenological equations are used in the work. These equations are not linear and approximate analytical solutions are found for them. The kinetics of destruction of previously experimentally detected dependencies on the preliminary treatment of a suspension with microorganisms by a pulsed electric field is described. The calculations were carried out taking into account the limited transparency of the bacterial cell wall. It is demonstrated that low permeability of the cell wall contributes to the survival of microorganisms in the aggressive environment. The dependence of the transparency of the cell wall on the influence of a pulsed electric field was found. In particular, the exponential dependence of transparency on the field amplitude is demonstrated. The calculation results are consistent with the experiment at a fixed value of the parameters. The agreement between theory and experiment in the entire range of voltage values for the amplitude of the electric field is available.

**Primary authors:** Mr YAKOVLIEV, Vladyslav (Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Kyiv); Dr ERMAKOV, Volodymyr (Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Kyiv)

**Presenter:** Mr YAKOVLIEV, Vladyslav (Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Kyiv)

**Session Classification:** Physics of Biological Macromolecules

**Track Classification:** Physics of Biological Macromolecules

Contribution ID: 24

Type: Oral

## First passage time distribution for spiking neuron with fast inhibitory feedback stimulated with renewal stream

Monday, 23 December 2019 17:05 (20 minutes)

We consider a class of spiking neuron models defined by a set of conditions typical for basic threshold-type models, such as leaky integrate-and-fire model and some artificial neurons. A series of impulses, representing a point renewal process, is applied to a neuron. Each output impulse is fed back to the neuron after a fixed time delay,  $\Delta$ . This impulse acts as an impulse received through a fast inhibitory (GABA<sub>A</sub>) synapse.

In our previous work [1], we have obtained a general relation in case of input Poisson stream for calculating exactly the probability density function (PDF)  $p(t)$  for the distribution of the first passage time of crossing the threshold.

In the present work, we have obtained a similar results but applicable in case of any renewal input stream. The calculation is based on the known PDF  $p^0(t)$  for the same neuron without feedback and the PDF of interspike intervals for input stream,  $p^{in}(t)$ .

[1]. Vidybida, A., Shchur, O. Relation between firing statistics of spiking neuron with delayed fast inhibitory feedback and without feedback, *Fluctuation and Noise Letters*, 17(01):1850005 (2018).

**Primary authors:** Ms SHCHUR, Olha (Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Kyiv); Dr VIDYBIDA, Alexander (Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Kyiv)

**Presenter:** Ms SHCHUR, Olha (Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Kyiv)

**Session Classification:** Statistical Theory of Many-body Systems

**Track Classification:** Statistical Theory of Many-body Systems

Contribution ID: 25

Type: **Poster**

## Spontaneous and engineered transformations of topological structures in nonlinear media with gain and loss

*Monday, 23 December 2019 17:50 (5 minutes)*

In contrast to conservative systems, in nonlinear media with gain and loss the dynamics of localized topological structures exhibit many unique features that can be controlled externally. We propose a robust mechanism to perform topological transformations changing characteristics of dissipative vortices and their complexes in a controllable way. We show that a properly chosen control carries out the evolution of dissipative structures to regime with spontaneous transformation of the topological excitations or drives generation of vortices with control over the topological charge.

**Primary authors:** Ms CHELPANOVA, Oksana (Taras Shevchenko National University of Kyiv); Dr YAKIMENKO, Oleksandr (Taras Shevchenko National University of Kyiv)

**Presenter:** Ms CHELPANOVA, Oksana (Taras Shevchenko National University of Kyiv)

**Session Classification:** Poster session

**Track Classification:** Condensed Matter Physics

Contribution ID: 26

Type: Poster

## Determination of the contact angle from transversality conditions of the Lagrange variation problem of wetting

Monday, 23 December 2019 17:55 (5 minutes)

In recent years, there has been an increase in studies focused on the size-dependent contact angle. In the case of the sessile axial symmetric droplet, the size dependence often is explained by the contribution of the line tension to the Helmholtz free energy as a consequence, the modified Young's equation. There are two major points of view on the contribution mechanism. According to the first point of view, the line tension is a function of the contact angle; according to another one, the line tension is a function of the three-phase contact line torsion and geodesic curvature. However, in the case of the straight contact line, it is impossible to determine the influence of the line tension of the three-phase contact line on the contact angle.

We propose a model of the line tension of the three-phase contact line influence on the contact angle. We consider the line tension as a thermodynamic work on the deformation transition region on the three-phase border to determine the influence. Therefore, the line tension becomes a function of the dividing surface curvature on the contact line. Then, the Helmholtz free energy of a unit of the cylindric nanodroplet length  $\Delta x$  with the additional condition of incompressibility of the nanodroplet liquid is:

$$F[z(y)] = \int_x^{x+\Delta x} dx \int_{-r}^r dy L(y, z, z', z'') = \int_x^{x+\Delta x} dx \int_{-r}^r dy \left\{ \gamma_{sv} - \gamma_{sl} + \gamma_{lv} \left[ \frac{z''^2}{(1+z'^2)^{3/2}} \right] \sqrt{1+z'^2} + \frac{1}{r} \tau \left[ \frac{z''^2}{(1+z'^2)^{3/2}} \right] + \lambda y z' \right\}, \quad (4)$$

where,  $2r$  – the width of the nanodroplet base,  $\gamma$  – the surface tension between liquid/vapor, solid/liquid and solid/vapor,  $\tau$  – the line tension of three-phase contact line,  $\lambda$  – Lagrange multiplier. The transversality conditions of the Lagrange problem with moving boundary for the functional containing the second-order derivative are:

$$\left[ L - z' \left( \frac{\partial L}{\partial z'} - \frac{d}{dy} \frac{\partial L}{\partial z''} \right) + \left( \frac{z' \arctan(z') (1+z'^2) - z'^2}{y (\arctan(z') - z')} - z'' \right) \frac{\partial L}{\partial z''} \right]_{y=-r, r} = 0. \quad (5)$$

The contact angle can be obtained by minimization of the Helmholtz free energy functional with the application of the transversality conditions:

$$\left( 1 - \left( \frac{\delta_c}{R} \right) + o \left( \frac{\delta_c}{R} \right)^2 \right) \cos(\theta) = \frac{\gamma_{sv} - \gamma_{sl}}{\gamma_{lv}^\infty} - \frac{\tau}{\gamma_{lv}^\infty R \sin(\theta)}, \quad (6)$$

where,  $\delta_c$  – the Tolman length,  $\theta$  – the contact angle,  $\gamma_{lv}^\infty$  – the surface tension of a flat surface,  $R$  – the radius of the liquid-vapor interface curvature.

It has been shown that the contact angle depends on the line tension of the straight three-phase contact line.

**Primary author:** Mr BURIAN, Sergii (Taras Shevchenko National University of Kyiv)

**Co-authors:** Mr HREBNOV, Oleh (Taras Shevchenko National University of Kyiv); Mr TYVONOVYCH, Ostep (Taras Shevchenko National University of Kyiv); Dr ISAEV, Mykola (Universite de Lorraine, CNRS, LEMTA)

**Presenter:** Mr HREBNOV, Oleh (Taras Shevchenko National University of Kyiv)

**Session Classification:** Poster session

**Track Classification:** Mathematical Physics

Contribution ID: 27

Type: **Oral**

## Backward nucleon production by heavy baryonic resonances in proton-nucleus collisions

*Tuesday, 24 December 2019 17:35 (20 minutes)*

The production of backward nucleons,  $N(180^\circ)$ , at  $180^\circ$  in the nuclear target rest frame in proton-nucleus ( $p + A$ ) collisions is studied. The backward nucleons appearing outside of the kinematically allowed range of proton-nucleon ( $p + N$ ) reactions are shown to be due to secondary reactions of heavy baryonic resonances produced inside the nucleus. Baryonic resonances  $R$  created in primary  $p + N$  reactions can change their masses and momenta due to successive collisions  $R + N \rightarrow R + N$  with other nuclear nucleons. Two distinct mechanisms and kinematic restrictions are studied: the reaction  $R + N \rightarrow N(180^\circ) + N$  and the resonance decay  $R \rightarrow N(180^\circ) + \pi$ . Simulations of  $p + A$  collisions using the Ultra-relativistic Quantum Molecular Dynamics model support these mechanisms and are consistent with available data on proton backward production.

**Primary author:** PANOVA, Oleksandra (Taras Shevchenko National University of Kyiv)

**Presenter:** PANOVA, Oleksandra (Taras Shevchenko National University of Kyiv)

**Session Classification:** Physics of Nuclei and Elementary Particles

**Track Classification:** Physics of Nuclei and Elementary Particles

Contribution ID: 28

Type: **Oral**

## **Bose gas with repulsive interactions between particles**

*Tuesday, 24 December 2019 17:15 (20 minutes)*

Bose-Einstein condensation (BEC) and particle number fluctuations are considered in the gas of bosons with repulsive interactions between particles. Two different mean-field models of the interacting Bose gas are studied. They provide rather different predictions for the BEC transition temperatures and the scaled variances of particle number fluctuations. The behavior of the BE condensate in the different versions of the mean-field approach is also investigated.

**Primary author:** BONDAR, Yehor (Taras Shevchenko National University of Kyiv)

**Presenter:** BONDAR, Yehor (Taras Shevchenko National University of Kyiv)

**Session Classification:** Physics of Nuclei and Elementary Particles

**Track Classification:** Physics of Nuclei and Elementary Particles

Contribution ID: 30

Type: **Oral**

## Traces of the nuclear liquid-gas phase transition in the analytic properties of hot QCD

*Tuesday, 24 December 2019 16:55 (20 minutes)*

The nuclear liquid-gas transition at normal nuclear densities,  $n \sim n_0 = 0.16 \text{ fm}^{-3}$ , and small temperatures,  $T \sim 20 \text{ MeV}$ , has a large influence on analytic properties of the QCD grand-canonical thermodynamic potential. A classical van der Waals equation is used to determine these unexpected features due to dense cold matter qualitatively. The existence of the nuclear matter critical point results in thermodynamic branch points, which are located at complex chemical potential values, for  $T > T_c \sim 20 \text{ MeV}$ , and exhibit a moderate model dependence up to rather large temperatures  $T \sim 100 \text{ MeV}$ . The behavior at higher temperatures is studied using the van der Waals hadron resonance gas (vdW-HRG) model. The baryon-baryon interactions have a decisive influence on the QCD thermodynamics close to  $\mu_B = 0$ . In particular, nuclear matter singularities limit the radius of convergence  $r_{\mu_B/T}$  of the Taylor expansion in  $\mu_B/T$ , with  $r_{\mu_B/T} \sim 2-3$  values at  $T \sim 140-170 \text{ MeV}$  obtained in the vdW-HRG model.

**Primary authors:** Prof. GORENSTEIN, Mark (Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Kyiv); POBEREZHNYUK, Roman (Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Kyiv); STOECKER, Horst (FIAS Goethe Universitaet Frankfurt GSI); VOVCHENKO, Volodymyr (Goethe University Frankfurt); Mr SAVCHUK, Oleh (Taras Shevchenko National University of Kyiv)

**Presenter:** Mr SAVCHUK, Oleh (Taras Shevchenko National University of Kyiv)

**Session Classification:** Physics of Nuclei and Elementary Particles

**Track Classification:** Physics of Nuclei and Elementary Particles

Contribution ID: 31

Type: **Oral**

## Nuclear critical point and fluctuations of conserved charges

*Tuesday, 24 December 2019 15:55 (20 minutes)*

The chemical freeze-out parameters in central nucleus-nucleus collisions are extracted consistently from hadron yield data within the quantum van der Waals (QvdW) hadron resonance gas model. The beam energy dependences for skewness and kurtosis of net baryon, net electric, and net strangeness charges are predicted. The QvdW interactions in asymmetric matter,  $Q/B \neq 0.5$ , between (anti)baryons yield a non-congruent liquid-gas phase transition, together with a nuclear critical point (CP) with critical temperature of  $T_c = 19.5$  MeV. The nuclear CP yields the collision energy dependence of the skewness and the kurtosis to both deviate significantly from the ideal hadron resonance gas baseline predictions even far away, in  $(T, \mu_B)$ -plane, from the CP. These predictions can readily be tested by STAR and NA61/SHINE Collaborations at the RHIC BNL and the SPS CERN, respectively, and by HADES at GSI. The results presented here offer a broad opportunity for the search for signals of phase transition in dense hadronic matter at the future NICA and FAIR high intensity facilities.

**Primary author:** POBEREZHZHNYUK, Roman (Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Kyiv)

**Presenter:** POBEREZHZHNYUK, Roman (Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Kyiv)

**Session Classification:** Physics of Nuclei and Elementary Particles

**Track Classification:** Physics of Nuclei and Elementary Particles

Contribution ID: 32

Type: **Oral**

## Embedded solitons in the double sine-Gordon lattice with next-neighbor interaction

*Monday, 23 December 2019 10:35 (20 minutes)*

Topological solitons under certain conditions can freely propagate without radiation in the discrete systems of Josephson junctions [1]. These solutions are known as embedded solitons [2]. The dynamics of soliton in the array of the small Josephson junctions which contain a ferromagnet (SFS, SFIS) in their structure and where the intercell inductance is taken into account is investigating. For such junctions the current-phase relation is complicated and the second harmonic must be considered. The possibility of embedded solitons existence in the array, where the inductive coupling between cells occurs not only between the nearest neighbors, but also with the subsequent ones is demonstrated [3]. These interactions can be either destructive or favorable for the embedded solitons creation. The equation of soliton motion in the array with long-range interaction is analytically obtained, the dispersion law for Josephson plasmons which essentially depends on the inductive interaction between the adjacent cells of the array is found. The simulation of soliton dynamics in such system performed, the range of system parameters and the set of velocities at which the embedded solitons existence is possible are obtained. The existence area is inversely proportional to the spectrum width of the linear waves that producing due to the soliton motion across the array. The influence of the array cells interaction parameters on the mode of the soliton free propagation is analyzed and the dependence of its velocity on these parameters is found. The current-voltage characteristics of the array with the signs of embedded solitons existence are constructed. The inaccessible voltage interval is formed on it, the upper edge of this interval is proportional to the sliding velocity of the embedded soliton and its size depends on the dissipation in the system.

[1]. M.Peyrard and M.D. Kruskal, *Physica D* 14, 88 (1984).

[2]. A. Champneys, B. Malomed, J. Yang and D. Kaup, *Physica D* 152-153, 340 (2001)

[3]. Yaroslav Zolotaryuk and Ivan O. Starodub, *Physical Review E* 100, 032216 (2019)

**Primary author:** STARODUB, Ivan O. (Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Kyiv)

**Co-author:** ZOLOTARYUK, Yaroslav (Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Kyiv)

**Presenter:** STARODUB, Ivan O. (Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Kyiv)

**Session Classification:** Condensed Matter Physics

**Track Classification:** Condensed Matter Physics

Contribution ID: 33

Type: **Oral**

## Effect of resonant impurity scattering of carriers on Drude peak broadening in uniaxially strained graphene

*Monday, 23 December 2019 12:35 (20 minutes)*

An explanation is proposed for the recently observed in optical spectra of monolayer graphene giant increase in the Drude-peak width under applied uniaxial strain. We argue that the underlying mechanism of this increase can be based on resonant scattering of carriers from inevitably present impurities such as adsorbed atoms that can be described by the Fano-Anderson model. We demonstrate that the often neglected scalar deformation potential plays the essential role in this process. The conditions necessary for the maximum effect of the giant Drude-peak broadening are determined. It is stressed that the effect is strongly enhanced when the Fermi level gets closer to the Dirac point. Our theoretical analysis provides guidelines for functionalizing graphene samples in a way that would allow to modulate efficiently the Drude-peak width by the applied strain.

**Primary author:** Mr SHUBNYI, V. O. (Bogolyubov Institute for Theoretical Physics Institute for Condensed Matter of the National Academy of Sciences of Ukraine, Kyiv)

**Co-authors:** Mr SHARAPOV, S. G. (Bogolyubov Institute for Theoretical Physics Institute for Condensed Matter of the National Academy of Sciences of Ukraine, Kyiv); SKRYPNYK, Y. V. (Bogolyubov Institute for Theoretical Physics Institute for Condensed Matter of the National Academy of Sciences of Ukraine, Kyiv); LOKTEV, V.M. (Bogolyubov Institute for Theoretical Physics Institute for Condensed Matter of the National Academy of Sciences of Ukraine, Kyiv\ National Technical University of Ukraine KPI, Kyiv)

**Presenter:** Mr SHUBNYI, V. O. (Bogolyubov Institute for Theoretical Physics Institute for Condensed Matter of the National Academy of Sciences of Ukraine, Kyiv)

**Session Classification:** Condensed Matter Physics

**Track Classification:** Condensed Matter Physics

Contribution ID: 34

Type: **Poster**

## DNN application for hydrodynamic task solution

*Monday, 23 December 2019 18:30 (5 minutes)*

The possibility of GPU usage combined with the substitution of numerical computations with the trained neural network for both relativistic and non-relativistic hydrodynamic equations yields the 104 - 106 performance boost compared to the standard numerical methods. The main idea behind the work starts from the fact that neural network is the so-called perceptron on the universal type. The deep sense behind this definition is that actually a neural network with one hidden layer can become the mapping of any type for smooth differentiable continuous functions. The trained Neural Network can as well perform the role of the time-dependent solution of the hydro-equations performing the regression and classification tasks for various types of hydro – solutions. The results of DNN application to the non-relativistic hydro problem are demonstrated for 1D and 2D cases. Further 3D generalization options and problems are discussed.

**Primary author:** TARADIY, Kirill (Frankfurt Institute for Advanced Studies, Frankfurt am Main, Germany)

**Presenter:** TARADIY, Kirill (Frankfurt Institute for Advanced Studies, Frankfurt am Main, Germany)

**Session Classification:** Poster session

**Track Classification:** Statistical Theory of Many-body Systems

Contribution ID: 35

Type: **Oral**

## Effective description of the frustrated Heisenberg three-leg and four-leg tubes in a strong magnetic field

*Monday, 23 December 2019 11:55 (20 minutes)*

We investigate the low-temperature properties of the spin-1/2 antiferromagnetic Heisenberg model on the frustrated three-leg [1-2] and four-leg [3-5] tubes with almost dispersionless (almost flat) lowest magnon band placed in an external magnetic field. The aim of our study is to develop a systematic theory of low-temperature high-field properties of the models by hand. Using standard operator perturbation theory and strong coupling approach, we construct low-energy effective Hamiltonians for three-leg and four-leg tubes, which are much simpler than the initial ones. Based on the effective-model description we examine the low-temperature properties of the considered frustrated quantum Heisenberg antiferromagnets in the high-field regime. To verify the region of the applicability of the obtained effective Hamiltonians we perform extensive exact diagonalization and density matrix renormalization group calculations and compare them with the results for the initial models.

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[2] J.-B. Fouet, et al., *Phys. Rev. B* **73**, 014409 (2006).

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[5] M. Arlego, et al., *Phys. Rev. B* **87**, 014412 (2013).

**Primary author:** Mrs KRUPNITSKA, Olesia (Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine, Lviv)

**Presenter:** Mrs KRUPNITSKA, Olesia (Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine, Lviv)

**Session Classification:** Condensed Matter Physics

**Track Classification:** Condensed Matter Physics

Contribution ID: 36

Type: Oral

## Quantum antiferromagnet in a magnetic field on frustrated kagome-lattice bilayer

*Monday, 23 December 2019 12:15 (20 minutes)*

We consider the spin-1/2 antiferromagnetic isotropic Heisenberg model on a kagome-lattice bilayer in the presence of an external magnetic field. We include an interlayer frustration term and study the case of ideal frustration when the nearest-neighbor intralayer interactions and the frustrating interlayer interactions are of the same strength. In this case, a completely dispersionless (flat) magnon band may become the lowest-energy one and we can use the localized-magnon picture to examine the system in more simple terms. In the vicinity of the saturation field, we map the low-energy states of the considered quantum system onto the spatial configurations of hard parallelograms on an auxiliary kagome lattice and face a much simpler problem of classical statistical mechanics. It allows us to construct an effective model and study the low-temperature thermodynamic properties of the original quantum model. Also, an effective model was constructed using perturbation theory.

**Primary author:** BALIHA, Vasyl (Institute for Condensed Matter of the National Academy of Sciences of Ukraine, Lviv)

**Presenter:** BALIHA, Vasyl (Institute for Condensed Matter of the National Academy of Sciences of Ukraine, Lviv)

**Session Classification:** Condensed Matter Physics

**Track Classification:** Condensed Matter Physics

Contribution ID: 37

Type: **Poster**

## Modelling of Spectral Energy Distribution from Protoplanetary Disk of IRAS 22150+6109

*Monday, 23 December 2019 18:15 (5 minutes)*

We present the result of modelling of spectral energy distribution of the infrared source IRAS 22150+6109. The object emits an excess of radiation in far infrared band. It was interpreted to be a young massive pre-main-sequence star and the protoplanetary disk on late stage. We use radiative transfer code RADMC-3D for the simulations of spectral energy distribution. The code itself implements the Monte-Carlo ray tracing method with spherical grid fragmentation. We performed simulations and obtained best-fit parameters for the model of the protoplanetary disk. The investigation of such objects will help to understand protoplanetary disks emission better.

**Primary authors:** BILINSKYI, Illia (Taras Shevchenko National University of Kyiv, Akademika Hlushkova Ave, 4, Kyiv, Ukraine, 03022); ZAKHOZHAY, Olga (Main Astronomical Observatory National Academy of Sciences of Ukraine); Dr BERCZIK, Peter (Main Astronomical Observatory National Academy of Sciences of Ukraine)

**Presenter:** BILINSKYI, Illia (Taras Shevchenko National University of Kyiv, Akademika Hlushkova Ave, 4, Kyiv, Ukraine, 03022)

**Session Classification:** Poster session

**Track Classification:** Astrophysics and Cosmology

Contribution ID: 38

Type: **Oral**

## Competitive interaction of hydrogen peroxide and water molecules with DNA recognition sites

*Monday, 23 December 2019 14:45 (20 minutes)*

Ion beam therapy is one of the most progressive methods in cancer treatment. Studies of water radiolysis process show that under the action of ionizing irradiation in the medium of biological cell different atomic and molecular species occur. The most long-living among them are hydrogen peroxide ( $\text{H}_2\text{O}_2$ ) molecules. But the role of hydrogen peroxide molecules in the deactivation of the DNA of cancer cells in ion beam therapy has not been determined yet.

In the present work competitive interaction of hydrogen peroxide and water molecules with atomic groups of non-specific (phosphate groups) and specific (nucleic bases) DNA recognition sites is investigated. Interaction energies and optimized spatial configurations of the considered molecular complexes are calculated with the help of atom-atom potential functions method and density functional theory. It is shown that hydrogen peroxide molecule can form a complex with  $\text{PO}_4$  group (with and without sodium counterion) that is more energetically stable than the same complex with water molecule. Also the atomic groups of Adenine, Thymine, Guanine and Cytosine that are more energetically favorable to be bound by  $\text{H}_2\text{O}_2$  rather than by  $\text{H}_2\text{O}$  molecule are determined. Moreover, spatial configurations of AT and GC base pairs stabilized much better by hydrogen peroxide rather than by water molecule are found. These configurations can occur on the pathways of opening of DNA base pairs during DNA unzipping experiments. Consequently, formation of such complexes can block genetic information transfer processes in cancer cells and can be a key factor during ion beam therapy treatment.

**Primary authors:** ZDOREVSKYI, Oleksii (Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Kyiv); Dr PIATNYTSKYI, Dmytro (Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Kyiv); Prof. VOLKOV, Sergey (Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Kyiv)

**Presenter:** ZDOREVSKYI, Oleksii (Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Kyiv)

**Session Classification:** Physics of Biological Macromolecules

**Track Classification:** Physics of Biological Macromolecules

Contribution ID: 39

Type: Oral

## Low-frequency vibrations of water molecules in the hydration spine of DNA minor groove

Monday, 23 December 2019 15:05 (20 minutes)

Under the natural conditions, DNA macromolecule takes the form of a double helix which structure is stabilized by water molecules and metal ions. The organization of the ion-hydration environment of the macromolecule depends on a region of the double helix. In particular, in the minor groove of the macromolecule the water molecules are highly structured and the spine of water molecules, bridging the N<sub>3</sub> atoms of purine and O<sub>2</sub> atoms of pyrimidine bases, is formed. The dynamics of water molecules in the DNA water spine should be characterized by the vibrations in the same spectra range as the conformational vibrations of DNA. Therefore, the goal of our study was the determination of distinctive vibration modes of water molecules in the DNA minor groove that may be observed in the low-frequency spectra. On the basis of the approach for the description of DNA conformational dynamics [2], the vibrational model has been elaborated. In the model the nucleosides are considered as physical pendulums, rotating around phosphate groups in the plane perpendicular to the helical axis, and water molecules are presented as the masses attached to physical pendulums in different pairs. The parameters of the model [2] and the results of molecular dynamics simulations [3] were used for the estimation of the frequencies and amplitudes of vibrations. As a result the mode of water translational vibrations in the hydrated spine of DNA minor groove has been established. This mode characterizes the displacements of water molecule as a single whole from the equilibrium position in the frequency range within 170 – 270 cm<sup>-1</sup>. The comparison of the obtained results with the experimental spectra of DNA in an aqueous environment showed that in this region of the vibrational spectra the translational vibrations of water molecules in the bulk phase as well as ion-phosphate vibrations of DNA are observed. Thus, the obtained results ground the presence of the mode of vibrations of water molecules in the hydration spine of the DNA minor groove among the modes of DNA conformational vibrations.

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**Primary authors:** Mrs BUBON, Tatyana (Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Kyiv); Dr PEREPELYTSYA, Sergiy (Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Kyiv)

**Presenter:** Mrs BUBON, Tatyana (Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Kyiv)

**Session Classification:** Physics of Biological Macromolecules

**Track Classification:** Physics of Biological Macromolecules

Contribution ID: 40

Type: **Poster**

## The Aharonov-Bohm effect and conic singularities for the Dirac equation

*Monday, 23 December 2019 18:05 (5 minutes)*

The solution of the problem of fermions scattering in one Aharonov-Bohm vortex involves constructing a one-parameter family of self-adjoint extensions. The Green function can be constructed from the corresponding solutions. The following is a comparison of quantum-mechanical scattering problem with quantum field theory problem on the search for correlation functions of fermion states. Namely, Green's function can be interpreted as correlation function in the space of fermion states. Also there is considered a similar problem about scattering of fermions on a conical singularity, which implies a similar analysis of the results.

**Primary author:** Mr NAICHUK, Eduard (Taras Shevchenko National University of Kyiv )

**Co-author:** Dr IORGOV, Nikolai (Bogolyubov Institute for Theoretical Physics)

**Presenter:** Mr NAICHUK, Eduard (Taras Shevchenko National University of Kyiv )

**Session Classification:** Poster session

**Track Classification:** Mathematical Physics

Contribution ID: 41

Type: **Poster**

## The covalent radii derived from the first-principle data

*Monday, 23 December 2019 18:20 (5 minutes)*

The concept of atomic covalent radius forms the basis for one of the simplest parameterizations for prediction of the covalent bond length and recovering molecular graphs from the set of interatomic distances. In the present contribution we adopt the recently proposed dataset [1] of covalent bond lengths resulting from the first-principle calculations to derive the covalent radii for H, B, C, N, O, F, Si, P, S, Cl, Ge, As, Se and Br elements within the additive covalent bond length model. The obtained first-principle covalent radii are shown to be in good agreements ones based on empirical data [2]. Availability of the large-size dataset of covalent bond lengths enabled the further analysis of errors in approximating the covalent bond length with the sum of the covalent radii. In particular, the effects of electronic conjugation and the chemical elements electronegativity difference were investigated [3].

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**Primary authors:** Mr CHUIKO, Valerii (Faculty of Physics of Taras Shevchenko National University of Kyiv); Mr NIKOLAIENKO, Tymofii (Faculty of Physics of Taras Shevchenko National University of Kyiv)

**Presenter:** Mr CHUIKO, Valerii (Faculty of Physics of Taras Shevchenko National University of Kyiv)

**Session Classification:** Poster session

**Track Classification:** Physics of Biological Macromolecules

Contribution ID: 42

Type: **Poster**

## Binding of antibiotic drug molecules to the surface of silver nanoparticles: tight-binding DFT study

*Monday, 23 December 2019 18:25 (5 minutes)*

Enhancement of therapeutic activity of organic drug molecules bound to nanoparticle surface has recently been highlighted as a possible way to overcome resistance of bacteria towards traditional antibiotics [1]. Investigation of the physical interactions responsible for such complexation, however, becomes challenging when nanoparticle is formed by transition metal atoms due to the need of accurate treatment of the nanoparticle polarizability [2]. Purely ab initio approaches, on the other hand, are typically ruled out by the number of atoms in such systems and consequent demands for computational resources. In the variety of molecular modeling approaches available nowadays, the density-functional based tight-binding (DFTB) method is unique in combining the clear hierarchy of physically sound approximations with high computational efficiency [3], thus, being ideal for treating the systems of hundreds of atoms in reasonable time.

In the present contribution we report the applications of DFTB-based automated conformational searching algorithms [4] to obtain the energetically most stable complexes formed by organic drug molecules Ceftriaxone and Doxorubicin with silver nanoparticles (ca. 1 nm diameter) of different shapes.

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**Primary authors:** Ms HUSAK, Olha (Faculty of Physics of Taras Shevchenko National University of Kyiv); Dr NIKOLAIENKO, Tymofii (Faculty of Physics of Taras Shevchenko National University of Kyiv); Dr PAVLENKO, Olena (Faculty of Physics of Taras Shevchenko National University of Kyiv)

**Presenter:** Ms HUSAK, Olha (Faculty of Physics of Taras Shevchenko National University of Kyiv)

**Session Classification:** Poster session

**Track Classification:** Physics of Biological Macromolecules

Contribution ID: 43

Type: **Oral**

## Scalar field dark matter with $\phi^6$ self-interaction

*Tuesday, 24 December 2019 11:55 (20 minutes)*

The ultralight dark matter (ULDM) model proposes as DM particles candidates bosons with typical mass  $10^{-22}$  eV, such that its de Broglie wavelength is of galactic scale ( $\sim$ kpc). The ULDM was among the models, that were proposed to resolve CDM tensions on the small scales, such as core-cusp and missing satellite problem. However last times it faces some difficulties between observed spiral galaxies rotation curves and the model's predictions, if one takes into account core/host halo mass relation and the relation between mass and radius of a central core, that follows from simulations. In the present work, we consider complex scalar field minimally coupled to gravity with  $\phi^6$  self-interaction potential. We will discuss this model's predictions including DM density distribution in the galactic halo and its potential regarding solving the above-mentioned problems.

**Primary author:** Ms KHELASHVILI, Mariia (Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Kyiv)

**Presenter:** Ms KHELASHVILI, Mariia (Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Kyiv)

**Session Classification:** Astrophysics and Cosmology

**Track Classification:** Astrophysics and Cosmology

Contribution ID: 44

Type: **Oral**

## **X-ray photoemission spectra for the Falicov-Kimball model with correlated hopping**

*Monday, 23 December 2019 11:35 (20 minutes)*

We present the results of the investigation of X-ray photoemission spectra (XPS) for the strongly correlated electron system with both local and nonlocal correlations (correlated hopping). We consider the Falicov–Kimball model, the simplest model of strongly correlated electrons, extended by the inclusion of the interaction with deep core-hole state. Despite its simplicity, the Falicov–Kimball model has a metal-insulator transition for large Coulomb repulsion and is exactly solvable via dynamical mean-field theory in infinite dimensions. XPS response at finite temperatures is connected with the core-hole propagator, which is exactly expressed by the functional determinants on the Keldysh contour in time domain.

Present study is a continuation of our previous works, which considered the effect of correlated hopping on thermal transport and optical spectra. As we found previously for a wide range of the correlated hopping parameters, there are some singularities on the single-particle density of states and on the transport function (“quasiparticle” scattering time). Due to these anomalies and violation of the electron-hole symmetry, there is a huge enhancement of the thermoelectric properties and optical conductivity exhibits a number of interesting features in the vicinity of these singularities. We show to what extent these anomalous features can be manifested on the X-ray photoemission spectra at finite temperatures.

**Primary author:** DOBUSHOVSKYI, Danylo (Institute for Condensed Matter of the National Academy of Sciences of Ukraine, Lviv)

**Presenter:** DOBUSHOVSKYI, Danylo (Institute for Condensed Matter of the National Academy of Sciences of Ukraine, Lviv)

**Session Classification:** Condensed Matter Physics

**Track Classification:** Condensed Matter Physics

Contribution ID: 45

Type: **Oral**

## Searching the warm dark matter signatures from Cosmic Dawn and Reionization epoch

*Tuesday, 24 December 2019 10:35 (20 minutes)*

The origin of dark matter (DM) is one of the most intriguing questions in modern physics. One of the most promising DM models is the so-called ‘warm’ dark matter (WDM) with particle mass in the range of keVs.

The signature of warm dark matter could be fewer small size dark matter halos and small mass galaxies in the early Universe (compared to the standard “cold dark matter” (CDM) scenario).

The Cosmic Dawn and Reionization epoch are an imprint of structure formation in the Universe, which depends both on the DM nature and baryonic processes. Therefore the study of this era may shed light on the properties of the dark matter particles as well as on the of baryonic processes during the formation of earliest structures in the Universe.

We analyze the different observational datasets about the Cosmic Dawn epoch and find that the thermal relic warm dark matter with particle mass  $\sim 2$  keV is in an agreement with these observations.

**Primary authors:** RUDAKOVSKYI, Anton (Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Kyiv); Dr IAKUBOVSKYI, Dmytro (Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Kyiv); SAVCHENKO, Denys (Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Kyiv); Dr TSIZH, Maxym (Ivan Franko National University of Lviv)

**Presenter:** RUDAKOVSKYI, Anton (Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Kyiv)

**Session Classification:** Astrophysics and Cosmology

**Track Classification:** Astrophysics and Cosmology

Contribution ID: 46

Type: **Oral**

## Thermodynamic properties of an interacting boson system

*Tuesday, 24 December 2019 16:35 (20 minutes)*

We consider the thermodynamical properties of an interacting boson system at finite temperatures and zero chemical potential within the framework of the Skyrme-like mean-field model. Self-consistency relations between the mean field and thermodynamic functions are derived. For illustration of our approach the thermodynamic properties of a  $\pi$ -meson system are investigated. We numerically solved the self-consistent equation for a particle density and derived all thermodynamical functions as functions of the temperature for different values of an attractive constant of coupling  $\kappa$ . It is shown that for some values of  $\kappa$  this system develops a first-order phase transition via formation of the Bose condensate at non-zero temperatures. Phase diagrams and the pressure  $p/T^4$ , energy density  $\epsilon/T^4$ , entropy density  $s/T^3$ , trace anomaly  $(\epsilon - 3p)/T^4$ , specific heat  $C_V/T^3$ , and the speed of sound  $c_s^2$  are calculated in the liquid-gas and condensed phases.

**Primary authors:** Mr ZHURAVEL, D. (Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Kyiv); Mr STASHKO, O.S. (Taras Shevchenko National University of Kyiv); Mr ANCHISHKIN, D.V. (Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Kyiv); Mr MISHUSTIN, I.N. (Frankfurt Institute for Advanced Studies, 60438 Frankfurt am Main, Germany/ National Research Center "Kurchatov Institute", 123182 Moscow, Russia); Mr STOCKER, H. (Frankfurt Institute for Advanced Studies, 60438 Frankfurt am Main, Germany/ Johann Wolfgang Goethe University, D-60438 Frankfurt am Main, Germany)

**Presenter:** Mr ZHURAVEL, D. (Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Kyiv)

**Session Classification:** Physics of Nuclei and Elementary Particles

Contribution ID: 47

Type: **Poster**

## Mathieu equation as a confluent Heun equation and its applications

*Monday, 23 December 2019 18:00 (5 minutes)*

Mathieu equation appears in different fields of physics and usually it's known as Schrodinger equation with cosine as potential but in more general sense it's a certain specification of confluent Heun equation. Heun equation is a second order ordinary differential equation with rational coefficients, with four regular singular points. Without loss of generality we can put these points in  $1, 0, t, \infty$ . In our work we consider Mathieu equation and confluent Heun equations and their connection with classical conformal blocks.

**Primary author:** Mr YANCHYSHEN, O.V. (Kyiv Academic University)

**Presenter:** Mr YANCHYSHEN, O.V. (Kyiv Academic University)

**Session Classification:** Poster session

**Track Classification:** Mathematical Physics

Contribution ID: 48

Type: **Oral**

## Transverse energy transfer by Alfvén waves in toroidal plasmas

Monday, 23 December 2019 16:05 (20 minutes)

Destabilized magnetohydrodynamic (MHD) eigenmodes can transfer the energy and momentum from the region where particles (e.g., fast ions) drive the plasma instability to another region, where the destabilized waves are damped. This phenomenon named “spatial channeling” (SC) was predicted in [1,2]. A key element of the SC is that the energy and momentum of particles driving the instability are transferred by the waves (eigenmodes), not by the diffusion or heat conduction. In this work the physics of the transverse energy transfer by Alfvén waves in toroidal plasmas is elucidated. It is found that, in contrast to the classical Alfvén waves in infinite plasmas, the Alfvén waves in toroidal systems produce plasma compression due to coupling with fast magnetoacoustic waves, which provides the energy transfer. The radial group velocities of the traveling waves constituting the Global Alfvén Eigenmodes and Toroidicity-induced Alfvén Eigenmodes are calculated. It is shown that equation for Alfvén eigenmodes derived in the approximation of vanishing wave field along the equilibrium magnetic field reproduce the longitudinal magnetic field of the wave and lead to correct transverse energy flux. The obtained results explain how Alfvén eigenmodes can provide the spatial energy channeling. The results of this work are published in [3]. This work was supported by the Project No. PL15/18 of the National Academy of Sciences of Ukraine and the Project No. 6392 of the Science and Technology Center in Ukraine (STCU).

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[3] Ya. I. Kolesnichenko, Yu. V. Yakovenko, and M. H. Tyshchenko, *Phys. Plasmas* **25**, 122508 (2018)

**Primary authors:** Mr KOLESNICHENKO, Ya. I. (Institute for Nuclear Research of the National Academy of Sciences of Ukraine, Kyiv); Mr YAKOVENKO, Yu. V. (Institute for Nuclear Research of the National Academy of Sciences of Ukraine, Kyiv); Mrs TYSHCHENKO, M.H. (Institute for Nuclear Research of the National Academy of Sciences of Ukraine, Kyiv)

**Presenter:** Mrs TYSHCHENKO, M.H. (Institute for Nuclear Research of the National Academy of Sciences of Ukraine, Kyiv)

**Session Classification:** Statistical Theory of Many-body Systems

**Track Classification:** Statistical Theory of Many-body Systems

Contribution ID: 49

Type: **Lecture**

## **Topological magnetic solitons in curvilinear nanomagnets**

*Monday, 23 December 2019 09:30 (45 minutes)*

**Primary author:** Mr KRAVCHUK, V.P. (Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Kyiv)

**Presenter:** Mr KRAVCHUK, V.P. (Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Kyiv)

**Session Classification:** Condensed Matter Physics

**Track Classification:** Condensed Matter Physics

Contribution ID: 50

Type: **Lecture**

## Epigenetics: "read" between DNA lines

*Monday, 23 December 2019 14:00 (45 minutes)*

**Primary author:** Mrs SHESTOPALOVA, A.V. (A.Ya. Usikov Institute for Radiophysics and Electronics National Academy of Sciences of Ukraine, Kharkiv)

**Presenter:** Mrs SHESTOPALOVA, A.V. (A.Ya. Usikov Institute for Radiophysics and Electronics National Academy of Sciences of Ukraine, Kharkiv)

**Session Classification:** Physics of Biological Macromolecules

**Track Classification:** Physics of Biological Macromolecules

Contribution ID: 51

Type: **Lecture**

## **Relaxation in classical integrable systems**

*Tuesday, 24 December 2019 13:30 (45 minutes)*

**Primary author:** Mr GAMAYUN, Oleksandr (University of Amsterdam)

**Presenter:** Mr GAMAYUN, Oleksandr (University of Amsterdam)

**Track Classification:** Mathematical Physics

Contribution ID: 52

Type: **Poster**

## Effects of parallel motion on test-particle transport

*Monday, 23 December 2019 18:35 (5 minutes)*

Transport processes play a significant role in the evolution of non-equilibrium plasmas. Various instabilities which exist in such plasma can generate intense fields that interact with particles and cause the anomalous transport. The intensity of the generated fields can be high enough to cause anomalous transport exceeding the collisional one. The possible explanation of a significant difference between anomalous and collisional transport characteristics is the particle trapping effect. The particle trapping effect is the crucial feature for a two-dimensional transport across the magnetic field, particularly when random electric field has an infinite correlation time. One of the common methods for a theoretical study of this problem is based on the Taylor relation combined with a certain statistical approximation of velocity correlation function along the trajectories. In our previous work we proposed and validated closure approximation [1] for an infinite correlation time and expanded it to account for finite Larmor radius effects [2] as well as finite correlation time [3]. However, it is also important to study the effect of the particle motion along the magnetic field on the particle transport.

Here we use numerical simulation to study three-dimensional particle motion in constant magnetic and random electric fields. A set of parameters, such as random field correlation time, finite Larmor radius and initial longitudinal velocity are considered. The effect of these parameters on particle transport are discussed.

This work is supported by the Project № 20-04/18-2019 of the National Academy of Sciences of Ukraine.

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**Primary author:** CHERNIAK, O.M. (Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Kyiv)

**Presenter:** CHERNIAK, O.M. (Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Kyiv)

**Session Classification:** Poster session

**Track Classification:** Statistical Theory of Many-body Systems