

**XII Conference of  
Young Scientists  
”Problems of  
Theoretical Physics”**

December 21 – 22, 2021

Bogolyubov Institute for Theoretical Physics

Kyiv, Ukraine

**Book of  
Abstracts**

## Tuesday, December 21

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**10-00**      **Conference opening**

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### Morning Session

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**10-05**      **Alexander K. Vidybida**

Lecture      “Physical mechanism of signal processing in biological neural networks”  
*Bogolyubov Institute for Theoretical Physics of the NAS of Ukraine,  
Kyiv, Ukraine*

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**10-50**      **Tymofii Nikolaienko**

O.1            “Approaching the atomic radii from in a data-oriented way: how can we  
benefit from a set of 'useless' structural properties?”  
*Taras Shevchenko National University of Kyiv, Kyiv, Ukraine*

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**11-10**      **Igor Gapyak**

O.2            “Propagation processes of correlations in the system of hard spheres”  
*Taras Shevchenko National University of Kyiv, Kyiv, Ukraine*

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**11-30**      **Liudmyla Sidletska, Oleg Gerasymov**

O.3            “Wave diagnostics of inhomogeneous inclusions in low-dimensional  
quasi-periodic structures”  
*Odesa State Environmental University, Odessa, Ukraine*

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**11-50**      **Dmytro Shapoval**

O.4            “Long-range hops in a two-species reaction-diffusion system:  
renormalization group and numerical simulations”  
*Institute of Condensed Matter Physics NAS of Ukraine, Doctoral  
College for the Statistical Physics of Complex Systems, Leipzig-  
Lorraine-Lviv-Coventry*

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**12-10**      **Marina Vorona**

O.5            “Pseudopotential method for description of positron annihilation in  
spherically symmetric potential”  
*Institute of Applied Physics NAS of Ukraine, Sumy, Ukraine*

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**12-30**      **LUNCH**

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## Afternoon Session

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- 14-00**      **Aleksandr Konstantinov**  
O.6          “The charge and the dipole moment of quantized vortex structures in superfluid systems”  
*B. Verkin Institute for Low Temperature Physics and Engineering, Kharkiv, Ukraine*
- 
- 14-20**      **Olesia Krupnitska**  
O.7          “Entanglement measures of a frustrated spin-1/2 Heisenberg octahedral chain within the localized-magnon approach”  
*Institute for Condensed Matter, NAS of Ukraine, Lviv*
- 
- 14-40**      **Roman Skorokhod**  
O.8          “The governing quantitative characteristics of radiation-induced segregation in Fe-Cr-Ni alloy”  
*Institute of Applied Physics NAS of Ukraine, Sumy, Ukraine*
- 
- 15-00**      **Artur Ovcharenko**  
O.9          “Calculation model of X-ray phase contrast image of tested structure”  
*Institute of Applied Physics NAS of Ukraine, Sumy, Ukraine*
- 
- 15-20**      **Yurii Zhuravlov**  
O.10        “Large time and long distance asymptotics of the thermal correlators of the impenetrable anyonic lattice gas”  
*Bogolyubov Institute for Theoretical Physics of the NAS of Ukraine, Kyiv, Ukraine*
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## Wednesday, December 22

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### Morning Session

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**10-00**      **Andrii Neronov**

Lecture

“Multimessenger astroparticle physics”

*Astronomy Department, University of Geneva & Université de Paris,  
CNRS, Astroparticule et Cosmologie*

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**10-45**      **Margarita Sobolenko, Peter Berczik, Rainer Spurzem, Manuel  
Arca Sedda, Francesco Paolo Rizzuto, Mirek Giersz,  
Konrad Maliszewski**

O.11

“Merging of spinning binary black holes in globular clusters”

*Main Astronomical Observatory the NAS of Ukraine, Kyiv, Ukraine*

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**11-05**      **Marina Ishchenko, Margaryta Sobolenko, Peter Berczik**

O.12

“Milky Way Globular Clusters: close encounter rates with each other  
and with the Central Supermassive Black Hole”

*Main Astronomical Observatory the NAS of Ukraine, Kyiv, Ukraine*

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**11-25**      **Kateryna Vovk**

O.13

“The new AGN search in SDSS «MaNGA» survey”

*Main Astronomical Observatory the NAS of Ukraine, Kyiv, Ukraine*

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**11-45**      **Edoardo Giangrandi, Violetta Sagun, Costança Providência,  
Tim Dietrich, Oleksii Ivanytskyi, K. A. Bugaev**

O.14

“Impact of asymmetric bosonic dark matter on neutron star properties”

*Centre for Physics of the University of Coimbra, Coimbra, Portugal*

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**12-05**      **Mykhaylo Lyashenko, Vyacheslav Kolodvazhnyi**

O.15

“Calculation of the values of the zonal component of the electric field  
and the velocity of transfer of the ionospheric plasma due to the  
electromagnetic drift during strong magnetic storms on  
October 12, 2021 and November 4, 2021”

*Institute of ionosphere, NAS and MES of Ukraine, Kharkiv, Ukraine*

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**12-30**      **LUNCH**

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### Afternoon Session

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- 13-30**      **Oleksii Ivanytskyi, David Blaschke**  
O.16      “Relativistic density functional approach to a unified description of  
quark-hadron matter”  
*Bogolyubov Institute for Theoretical Physics, NAS of Ukraine, Kyiv*
- 
- 13-50**      **Nursultan Kalzhigitov**  
O.17      “Influence of cluster polarization on spectrum and elastic processes in <sup>6</sup>LI”  
*Al-Farabi Kazakh National University, Almaty, Republic of Kazakhstan*
- 
- 14-10**      **Roman Poberezhnyuk, Oleksandr Stashko, Oleh Savchuk,**  
              **Volodymyr Vovchenko, Mark Gorenstein**  
O.18      “Phase diagram of interacting pion matter and isospin charge  
fluctuations”  
*Bogolyubov Institute for Theoretical Physics, NAS of Ukraine, Kyiv*
- 
- 14-30**      **Oleh Savchuk, Volodymyr Vovchenko, Volker Koch,**  
              **Horst Stoecker, Jan Steinheimer**  
O.19      “Constraining baryon annihilation in the hadronic phase of heavy-ion  
collisions via event-by-event fluctuations”  
*Bogolyubov Institute for Theoretical Physics, NAS of Ukraine, Kyiv*
- 
- 14-50**      **Vladimir Kuznietsov, Oleh Savchuk, Oleksandr Stashko,**  
              **Mark Gorenstein**  
O.20      “Critical point and Bose-Einstein condensation in pion matter”  
*Taras Shevchenko National University of Kyiv, Kyiv, Ukraine*
- 
- 15-10**      **Volodymyr Shapoval, Yuri Sinyukov**  
O.21      “The estimation of pion and kaon maximal emission times in 5.02A TeV  
collisions at the LHC”  
*Bogolyubov Institute for Theoretical Physics of the NAS of Ukraine,  
Kyiv, Ukraine*
- 
- 15-30**      **Musfer Adzhymambetov, Yuri Sinyukov**  
O.22      “First results of iHKM at RHIC BES energies: measuring shear viscosity  
of QGP ”  
*Bogolyubov Institute for Theoretical Physics of the NAS of Ukraine,  
Kyiv, Ukraine*
- 
- 15-50**      *Closing of the conference*

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## Physics of Biological Macromolecules

# Approaching the atomic radii from in a data-oriented way: how can we benefit from a set of 'useless' structural properties?

**Authors:** Tymofii Nikolaienko<sup>1</sup>; Leonid Bulavin<sup>1</sup>

<sup>1</sup> *Taras Shevchenko National University of Kyiv*

We report utilization of a collection of interatomic distances, obtained from 28 710 molecules after optimizing their geometries with quantum-chemical methods, to introduce a new set of atomic radii for H, B, C, N, O, F, Si, P, S, Cl, Ge, As, Se, Br elements. This problem is tackled from a perspective which differs significantly from many conventional approaches, like van der Waals radii or the covalent ones, which typically focus on introducing the atomic radii as the descriptors tailored for modeling specific sort of atomic contacts or bonded states found in diatomic fragments respectively. In contrast to that, we study the possibility of finding the atomic radii as parameters of a linear machine-learned binary classifier, trained to distinguish between bonded and non-bonded pairs of atoms [1]. We demonstrate, that although the distances between non-bonded atomic pairs play an essential role in training this classifier, the obtained radii still exhibit considerable similarities to the conventional covalent ones [2]. We thereby provide an example for how a proper data-oriented treatment can turn seemingly useless data into the useful one. Additional details on the procedure [3] used to create a dataset of interatomic distances in fully automated, yet chemically sound manner, are discussed.

## References

- [1] T.Y. Nikolaienko and L.A. Bulavin, *Comput. Theor. Chem.* (2021), 1204: 113389.
- [2] T.Y. Nikolaienko, V.S. Chuiko and L.A. Bulavin, *Mol. Phys.* (2020), **118**: e1742937.
- [3] T.Y. Nikolaienko, V.S. Chuiko and L.A. Bulavin, *Comput. Theor. Chem.* (2019), **1163**: 112508.

## **Statistical Theory of Many-body Systems**

# **Propagation processes of correlations in the system of hard spheres**

**Author:** Igor Gapyak<sup>1</sup>

<sup>1</sup> *Taras Shevchenko National University of Kyiv*

In this talk we consider an approach to the description of the evolution of a state by means of both reduced distribution functions and reduced correlation functions, which is based on the dynamics of correlations in a system of hard spheres. It should be emphasized that the generating operators of solution expansions of the corresponding hierarchies of evolution equations are induced by the generating operators of an expansion of the Liouville hierarchy solution for a sequence of correlation functions.

In the talk an approach to the description of the state evolution of a system of hard spheres by means of the state of a typical particle determined by the generalized Enskog equation is also discussed or, in other words, the foundations of the correlations evolution description by kinetic equations are considered.

## Statistical Theory of Many-body Systems

# Wave diagnostics of inhomogeneous inclusions in low-dimensional quasi-periodic structures

**Authors:** Liudmyla Sidletska<sup>1</sup>; Oleg Gerasymov<sup>1</sup>

<sup>1</sup> *Odessa State Environmental University*

In the classical work Rayleigh showed that a plane wave propagating in a one-dimensional periodic unbounded structure, for some wavelengths, undergoes total reflection at the boundaries of a fragment, called in the modern terminology accepted in the theory of such structures, called photonic crystals, a forbidden band. In this case (by the Bloch – Floquet theorem) the wave amplitude inside the periodic system decays exponentially [1].

In this paper, we consider a quasi-one-dimensional, semi-bounded layered periodic structure, in which the first (in order) layer has characteristics (refractive index, dielectric constant) that differ from other elements. We postulate that such a construction can serve as a model, for example, of a granular chain starting from an isotopic defect (or from an impurity particle).

In this work, a criterion is established for the condensation of the spectrum near one of the boundaries of the forbidden zone corresponding to the non-propagating wave mode. In a real prototype, a granular chain, such a mode (for example, in an electromagnetic wave) is, as it were, "arrested" in a certain vicinity of the impurity.

As a result, it was demonstrated how, when the symmetry of the initial state of the system is violated, say, due to the formation of defects (or deterministic incorporation of impurities), it is possible to form exponentially growing and decaying modes with the formation of a separate one localized in the vicinity of the defect. The established regularities can be used as the basis for wave diagnostics of impurity inclusions, as well as defects in quasi-one-dimensional quasi-periodic physical systems, for example, inhomogeneous low-dimensional crystal structures operating on the principle of a wave diode [2].

[1] P.G. Kevrekidis. Non-linear waves in lattices: Past, present, future. IMA J. Appl. Math. 2011. V. 76 (3). P. 389-423; <https://doi.org/10.1093/imamat/hxr015>

[2] S. Kasap, H. Ruda, Y. Boucher. Cambridge Illustrated Handbook of Optoelectronics and Photonics. - Cambridge, 2009 . P. 352

## Statistical Theory of Many-body Systems

# Long-range hops in a two-species reaction-diffusion system: renormalization group and numerical simulations

Authors: Dmytro Shapoval<sup>1</sup>; Viktoria Blavatska<sup>1</sup>; Maxym Dudka<sup>1</sup>

<sup>1</sup> *Institute of Condensed Matter Physics, National Academy of Sciences of Ukraine*  
<sup>1,4</sup> *Collaboration & Doctoral College for the Statistical Physics of Complex Systems, Leipzig-Lorraine-Lviv-Coventry*

We consider the reaction-diffusion system of two-species with an anomalous superdiffusion undergoing the annihilation and coagulation reactions  $A + A \rightarrow (0, A)$  as well as the trapping reaction  $A + B \rightarrow A$ . The superdiffusion is modeled via long-ranged Lévy flights represented by random walks with step-lengths obeying a Lévy distribution  $P(r) = r^{-d-\sigma}$  (a heavy-tailed probability distribution) with control parameter  $0 < \sigma \leq 2$ . This system for the case of the ordinary diffusing Brownian particles is known to demonstrate scaling of particle density and density correlation function of target particles  $B$  with nontrivial universal exponents including anomalous dimension for  $d \leq d_c$  (fluctuation-dominated kinetics), where  $d_c = 2$  is the upper critical dimension [1, 2].

It is well-known, that replacing the diffusive propagation with long-ranged Lévy flights modifies the dynamics of reactive systems [3]. Moreover, when the diffusion is anomalous as when the particles perform such Lévy flights, the upper critical dimension depends on the Lévy index  $\sigma$  [3, 4]. We are interested in the question how superdiffusion modifies the scaling of observable quantities below the upper critical dimension  $d \leq d_c = \sigma$ . We have applied the renormalization group formalism [5] for the system under study and calculated the decay exponents of the particle density as well as the density correlation function in the case of the Lévy flights. We have performed the numerical simulations of the studied system as well, obtained quantitative estimates for the decay exponents are in good agreement with our analytical results [6].

- [1] R. Rajesh, O. Zaboronski, *Phys. Rev. E* **70**, 036111 (2004)
- [2] B. Vollmayr-Lee, J. Hanson, R.S. McIsaac, J.D. Hellerick, *J. Phys. A: Math. Theor.* **51**, 034002 (2018); *ibid.* **53**, 179501 (2020)
- [3] H. Hinrichsen and M. Howard, *Eur. Phys. J. B* **7** 635 (1999)
- [4] D. C. Vernon, *Phys. Rev. E* **68** 041103 (2003)
- [5] U. C. Täuber, *Critical Dynamics: A Field Theory Approach to Equilibrium and Non-Equilibrium Scaling Behavior* (Cambridge University Press, Cambridge, 2014)
- [6] D. Shapoval, V. Blavatska, M. Dudka, *in preparation* (2021).

## Statistical Theory of Many-body Systems

# Pseudopotential method for description of positron annihilation in spherically symmetric potential

**Authors:** Marina Vorona<sup>1</sup>; Oleksandr Lebed<sup>1</sup>

<sup>1</sup> *Institute of Applied Physics NAS of Ukraine, Sumy, Ukraine*

The radiation resistance is the key issue for the creation of new structural elements for new-generation nuclear reactors and the operation extension of existing nuclear power plants. The study of the mechanisms of formation and dynamics of radiation defects is of considerable scientific interest. The initial stage of the evolution of radiation defects is the production of point-type defects. One of the most effective methods for studying point defects is spectroscopy of positron lifetime, which depends on the electron distribution. Despite the rather simple idea, its practical implementation is associated with both certain technical difficulties, and the development of a general process theory. The method of positron annihilation spectroscopy (PAS) includes measurement of positron lifetime, determination of probabilities of  $3\gamma$  and  $2\gamma$  positron annihilation, influence on the main characteristics of annihilation of various external factors [1-3]. The PAS method is used to study the electron structure of the material and the concentrations of point and extended defects. Local formations (defects) are characterized by reduction of electron density compared to defect-free regions, so the lifetime of the positron is longer in this defect. Each defect is corresponded its own lifetime and the intensity of the corresponding component in the total experimental spectrum, which determined by the concentration of such defects [1-3]. The positron annihilation rate is determined by the overlap of the electron and positron densities in the region of the positron localization. It also depends on the cross section of the electron-positron pair annihilation process.

A series of methods have been developed to study the electronic structure of matter. They all have their advantages and disadvantages and differ in the required initial data. For this problem, we considered the pseudopotential method, which allows us to build the potential of the positron-vacancy interaction. The method idea suppose the replacement of the atom potential by a weak potential with the same amplitude of conduction electrons scattering. The method is based on the factorization of the positron wave function into an energy-independent basic function and the smooth envelope (pseudo-wave) function. Thus, the annihilation process of the positron in a spherically symmetric potential can be described.

- [1]. West, R. N. Positron Studies of Lattice Defects in Metals. Positrons in Solids, 1979, p. 89-144.
- [2]. Puska M.J., Nieminen R.M. .. Theory of positrons in solids and on solid surfaces // Reviews of Modern Physics. 1994, v. 66, p. 841-897.
- [3]. Grafutin I., Prokopyev E.P. Application of positron annihilation spectroscopy to study the structure of matter, Physics-Uspekhi (2002),45(1):59.

## Condensed Matter Physics

# The charge and the dipole moment of quantized vortex structures in superfluid systems

**Authors:** Aleksandr Konstantinov<sup>1</sup>; Sergey Shevchenko<sup>1</sup>

<sup>1</sup> *B.Verkin Institute for Low Temperature Physics and Engineering of the National Academy of Sciences of Ukraine*

The problem of the electric fields created outside a superfluid liquid when quantum vortices and vortex rings appear inside the system is solved. It is shown that in the presence of a magnetic field a quantum vortex line acquires a linear charge density. The value of the charge density depends on the angle between the circulation vector and the magnetic field. It was found that a charge is associated with a rectilinear vortex filament, and a dipole moment is associated with a vortex ring. It was found that the key role while observing of electric fields outside the system is played by the shape of the surface that bounds the superfluid system. It was established that the polarization associated with the velocity field of the vortex ring does not cause the appearance of an electric field outside an infinite cylindrical capillary with a circular cross section in the case when the capillary axis coincides with the ring axis. If the system does not have such a high symmetry and the axis of the ring does not coincide with the axis of the capillary, the electric field outside the system is nonzero. The considered vortex structures can be generated by flows and can be associated with the transition of the system to a quantum turbulent state. For a laminar counterflow state of a superfluid system in a cylindrical circular capillary the electric potential outside the system is identically equal to zero [1,2]. Therefore, the predicted magneto-electric properties of quantum vortex structures can serve as a basis for creating a sensitive quantum turbulent state detector for superfluid systems.

[1] S. I. Shevchenko and A. M. Konstantinov, JETP Letters, 109, 790 (2019).

[2] S. I. Shevchenko and A. M. Konstantinov, Low Temp. Phys. 46, 48 (2020).

## Condensed Matter Physics

# Entanglement measures of a frustrated spin-1/2 Heisenberg octahedral chain within the localized-magnon approach

**Author:** Olesia Krupnitska<sup>1</sup>

<sup>1</sup> *Institute for Condensed Matter Physics, NAS of Ukraine*

We consider the spin-1/2 antiferromagnetic Heisenberg model on the frustrated octahedral chain in a presence of the external magnetic field. In a previous study [1], it was shown that the localized-magnon theory [2] can be modified for simpler calculation of concurrence [3], which may serve as a measure of the bipartite entanglement between nearest-neighbor and next-nearest-neighbor spins on squares of the octahedral chain. The results presented in [1] confirmed a new paradigm of the localized-magnons concept concerned with a simple calculation of entanglement measure. This study is devoted to further application of a modified localized-magnon theory for finding other entanglement measures. To be specific, we will consider such measures of entanglement as entanglement of formation and negativity [4-5]. It could be, thus, concluded that the localized-magnon theory can be straightforwardly adapted in order to calculate the respective entanglement measures for a wide class of flat-band quantum Heisenberg antiferromagnets.

[1] J. Strecka, O. Krupnitska and J. Richter, *EPL*, **132** 30004 (2020).

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

[3] L. Amico et al., *Rev. Mod. Phys.* **80**, 517 (2008).

[4] A. Peres, *Phys. Rev. Lett.* **77**, 1413 (1996).

[5] G. Vidal and R.F. Werner, *Phys. Rev. A* **65**, 032314 (2002).

## Condensed Matter Physics

# The governing quantitative characteristics of radiation-induced segregation in Fe-Cr-Ni alloy

**Authors:** Roman Skorokhod<sup>1</sup>; Oleksandr Koropov<sup>1</sup>

<sup>1</sup> *Institute of Applied Physics of National Academy of Sciences of Ukraine, Sumy, Ukraine*

A profound consequence of irradiation (neutron, proton, electron and heavy ion) of metal alloys is the spatial redistribution of alloy components. As a result, there are enrichment or depletion of the main, solute and impurity components of the alloy near the defect sinks. This phenomenon is called radiation-induced segregation (RIS) and leads to degradation of mechanical and physicochemical properties of materials.

The spatial and temporal evolution of the concentrations of alloy components  $C_k$  ( $k = \text{Fe, Cr, Ni}$ ) and point defects (PD) (vacancies  $C_v$  and interstitials  $C_i$ ) in the ternary concentrated Fe-Cr-Ni alloys under irradiation is described by the system of five coupled nonlinear partial differential equations [1-3]:

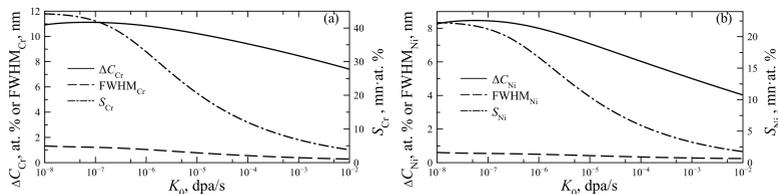
$$\begin{cases} \frac{\partial C_k}{\partial t} = -\nabla \mathbf{J}_k, \\ \frac{\partial C_v}{\partial t} = -\nabla \mathbf{J}_v + K_0 - R_{iv} C_v C_i - k_v^2 D_v (C_v - C_v^{eq}), \\ \frac{\partial C_i}{\partial t} = -\nabla \mathbf{J}_i + K_0 - R_{iv} C_v C_i - k_i^2 D_i (C_i - C_i^{eq}). \end{cases} \quad (1)$$

where the fluxes of atoms species  $k$  is  $\mathbf{J}_k$ , vacancies  $\mathbf{J}_v$  and interstitial  $\mathbf{J}_i$  defined as:

$$\mathbf{J}_k = - \left( \sum_{d=v,i} d_{k,d} C_d \right) \nabla C_k + C_k (d_{k,v} \nabla C_v - d_{k,i} \nabla C_i), \quad (2)$$

$$\mathbf{J}_v = - \sum_{k=\text{Fe, Cr, Ni}} d_{k,v} C_k \nabla C_v + \alpha C_v \left( \sum_{k=\text{Fe, Cr, Ni}} d_{k,v} \nabla C_k \right), \quad (3)$$

$$\mathbf{J}_i = - \sum_{k=\text{Fe, Cr, Ni}} d_{k,i} C_k \nabla C_i - \alpha C_i \left( \sum_{k=\text{Fe, Cr, Ni}} d_{k,i} \nabla C_k \right), \quad (4)$$



**Figure 1:** Production rate dependence of surface Cr depletion  $\Delta C_{Cr}$  and Ni enrichment  $\Delta C_{Ni}$  (solid line),  $FWHM_{Cr}$  and  $FWHM_{Ni}$  (dashed line) and segregation area of Cr  $S_{Cr}$  and Ni  $S_{Ni}$  (dash-dotted line). Calculations were performed at temperature  $T = 400\text{--}600\text{ }^{\circ}\text{C}$ , dose  $D = 10\text{-dpa}$  (displacement per atom).

$K_0$  is the production rate of radiation PD,  $R_{iv}$  is the recombination rate of PD,  $k_v^2$  and  $k_i^2$  are the sink strengths for vacancies and interstitials respectively,  $C_v^{eq}$  and  $C_i^{eq}$  are the equilibrium vacancy and interstitial concentrations,  $D_v$  and  $D_i$  are the diffusion coefficients of vacancies and interstitial,  $d_{k,v}$  and  $d_{k,i}$  are the diffusivity coefficients of vacancies and interstitial. The system with the corresponding initial and boundary conditions is solved numerically (a detailed solution algorithm is given in [2]).

The aim of the present paper is to calculate the governing quantitative characteristics of RIS for Fe-20%Cr-8%Ni alloy under the irradiation. That are: concentration profiles of atoms species  $k$   $C_k(x)$  and PD  $C_{v(i)}(x)$ , surface concentration of atoms species  $k$   $C_k^{surf}$ , the value of surface enrichment (depletion) of atoms species  $k$   $\Delta C_k$ , the full width of the concentration profile of atoms species  $k$  at half maximum enrichment (depletion)  $FWHM_k$ , segregation area of atoms species  $k$   $S_k$  and discriminant of RIS of atoms species  $k$  in a steady state  $\mathcal{D}_k$ . For example, production rate dependence of surface depletion, FWHM and segregation area for Cr and Ni are shown in Fig. 1.

The Authors acknowledge the support by the target research program of National Academy of Sciences of Ukraine “Nuclear and radiation technologies for the energy sector and social needs” for 2019-2023.

[1]. Was G.S. Fundamentals of Radiation Materials Science: Metals and Alloys (2nd ed.). New York: Springer-Verlag, 2017. 1002 p.

[2]. Skorokhod R.V., Koropov A.V. Modeling of Radiation-Induced Segregation in Fe–Cr–Ni Alloys. Physics of the Solid State. 2019. Vol. 61, P. 2269–2276.

[3]. Koropov O.V., Skorokhod R.V., in Proceedings of Ninth International Scientific-Practical Conference “Mathematics in Modern Technical University”, Kyiv, December, 28–29, 2020. Vinnytsia: Publisher FOP Kushnir Yu. V., 2021. P. 80-89. (in Ukrainian)

## Mathematical Physics

# Calculation model of X-ray phase contrast image of tested structure

**Author:** Artur Ovcharenko<sup>1</sup>

**Co-author:** Oleksandr Lebed<sup>1</sup>

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The X-ray phase contrast imaging (PCI) method allows to visualize the internal structure of objects with small density gradients with high spatial resolution. The PCI technique is based on the use of the phenomenon of X-ray refraction, which leads to a change in the phase front of the wave that passed through the sample. As a result of such deformation of the phase front X-rays deviate from their primary direction at small angles, the magnitude of which depends on the spatial distribution of the density of matter in the object under study [1]. The phase shift of X-rays can't be measured directly, so it is converted into a intensity difference by specified ways that it can be detected. PCI technique can also be combined with tomographic methods to obtain a 3D-distribution of the refractive index in the sample.

In the presented research the calculation methods are considered for the diffraction result on the test structure. Each of sections of this structure changes the phase of the incident radiation in a specified manner. Due to the fact that Fraunhofer diffraction is observed at a considerable distance between source and screen, it is one of the limit cases of the scalar Kirchhoff diffraction theory. A one-dimensional case of diffraction was considered at first, where a linear phase change occurred within each of the lattice periods. As shown by the calculations for the phase lattice, the obtained intensity distribution differs qualitatively from the previously considered case of the amplitude lattice. Thus, one can see the displacement of the position of the central maximum distribution for case of a phase grating relatively the initial position. Due to this, the possibility is achieved for incident radiation concentrating in the chosen position. Graphs of intensity distribution for different indicator of linear phase change, as well as for different sizes of inhomogeneous section in the periodic structure of the phase lattice are calculated [2]. The peculiarities of the intensity distribution of diffracted radiation for such test objects are shown.

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## Mathematical Physics

# Large time and long distance asymptotics of the thermal correlators of the impenetrable anyonic lattice gas

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We study thermal correlation functions of the one-dimensional impenetrable lattice anyons. These correlation functions can be presented as a difference of two Fredholm determinants. To describe large time and long distance behavior of these objects we use effective form factor approach. The asymptotic behavior is different in the space-like and time-like regions. In particular, in the time-like region we observe the additional power factor on top of the exponential decay. We argue that this result is universal as it is related to the discontinuous behavior of the phase shift function of the effective fermions. At particular values of the anyonic parameter we recover asymptotics of spin-spin correlation functions in XXO quantum chain.

## Astrophysics and Cosmology

# Merging of spinning binary black holes in globular clusters

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Currently over 50 gravitational events from compact binaries were reported by LIGO-Virgo consortium. We see Gravitational Waves (GW) as a new and very powerful informational channel. The current GW observations contain the Binary Black Hole (BH) systems key orbital parameters, such as mass, semi-major axis, eccentricity and even the possible spins of the BH's. The next 3G generation of ground-based observatories (Einstein Telescope, Cosmic Explorer) will have the opportunity to work with GWs during multiple cycles. It can significantly improve the estimations of individual components parameters of BH's. Based on our current high resolution direct N-body modelling of the Milky Way typical Star Cluster systems dynamical evolution we try to numerically estimate the influence of individual spins values, orientations and orbital eccentricities on GW waveforms and observed time-frequency maps during multiple cycles for BH binary mergers. In our, up to date, N-body dynamical simulations we use the high order relativistic post-Newtonian corrections for the BH binary particles (3.5 post-Newtonian (PN) terms including spin-spin and spin-orbit terms). In the current work we present the GW waveforms catalogue which covers the large parameter space in mass ratios 0.05 - 0.82 and extreme possible individual spin cases.

## Astrophysics and Cosmology

# Milky Way Globular Clusters: close encounter rates with each other and with the Central Supermassive Black Hole

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The recent precise astrometric measurements by Gaia Data Release 2 (DR2) provide a possibility to measure the mean proper motions for the large sample of (~150) GCs of the Milky Way (MW), which makes it plausible to study the orbital evolution of the globular clusters (GCs) system as the whole. To explore the possible close encounters (i.e., possible collisions) between the GCs and Central Black Hole (CBH), we performed the orbital calculations in total of 152 GCs using our self-developed high-order  $\phi$ -GRAPE code. We integrated (up to 10 Gyr in look-back time) the orbits of objects with reliable positions and proper motions in five different external gravitational potential models. They were selected from Illustris TNG-100 cosmological simulation and have a variable in time mass, and sizes. Using complex criteria on impact factors, half-mass radii and relative velocity for the collision's detection, we found approximately 45 pairs of possible GCs "collisions" for all the five external potential models. We estimated 6 close encounter events with CBH on separations less than 100 pc from the center. The GCs sample consists of NGC 6121, NGC 6544, NGC 6642 passed close in all systems with five potential models; Terzan 9 and NGC 6981 - in systems with four potential models (not fully crossing); Pal 2 - in systems with two potential models.

**Astrophysics and Cosmology**

**The new AGN search in SDSS «MaNGA» survey**

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Aiming for searching outflows in AGN host' plane a sample of ~600 galaxies was created from SDSS Marvin 16th Data release. Profiles of [OIII]5007AA spectrum line were investigated by fitting two, three or four Gaussians. With significance of more then 3-sigma complicated gaseous movements in some AGN hosts were revealed. The frequency of different outflow structures were estimated.

## Astrophysics and Cosmology

# Impact of asymmetric bosonic dark matter on neutron star properties

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We study an accumulation of asymmetric bosonic dark matter inside neutron stars and its further impact on star's evolution. We present the conditions at which dark matter particles tend to condensate in a core of the star or create an extended halo. We show that dark matter condensed in a core leads to a decrease of the total gravitational mass and tidal deformability compared to a pure baryonic star. In addition, at some conditions self-gravitating dark matter can collapse gravitationally and form a black hole that can destroy the star. We study the range of particle mass, coupling constant and fraction of dark matter inside the neutron star that lead to the formation of a black hole inside a compact star. By imposing an existing astrophysical and gravitational wave constraints we set a new limit on the mass and fraction of dark matter particles.

## Astrophysics and Cosmology

## Calculation of the values of the zonal component of the electric field and the velocity of transfer of the ionospheric plasma due to the electromagnetic drift during strong magnetic storms on October 12, 2021 and November 4, 2021

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It is well known that, under quiet geomagnetic conditions, the contribution of magnetospheric sources to electric fields and currents at middle and low latitudes is small. Under undisturbed conditions, the magnitude of the zonal component of the electric field is several units of  $mV/m$ . Plasma transport in the ionosphere caused by these fields plays an insignificant role in contrast to plasma transport due to ambipolar diffusion and neutral (thermospheric) winds. However, during magnetic storms, the penetration of electric fields to the heights of the ionosphere of middle latitudes takes place and, as a consequence, an increase in the plasma velocity is observed due to the electromagnetic drift  $v_{EB}$ . In turn, an increase in  $v_{EB}$  leads to variations in the neutral wind velocity and, as a consequence, to a change in the parameters of the global thermospheric circulation. Such a change in the dynamic mode of the ionospheric plasma significantly affects the altitude distribution of the ionospheric parameters.

The aim of this work is to estimate the magnitude of the zonal component of the electric field in the ionosphere over Central Europe during strong magnetic storms on October 12 and November 4, 2021, as well as to calculate the velocity of plasma transfer in crossed electric and magnetic fields.

The behavior of the ionospheric parameters was analyzed and the values of the zonal component of the electric field  $E_y$  and the velocity of plasma transport due to the electromagnetic drift  $v_{EB}$  were estimated during two strong magnetic storms on October 12, 2021 ( $Kp_{max} = 6$ ,  $D_{st} = -64$  nT) and November 4, 2021 ( $Kp_{max} = 7$ ,  $D_{st} = -115$  nT).

During the magnetic storm on October 12, 2021, the maximum value of  $|E_y|$  was equal to  $27$  mV/m, and the drift velocity  $v_{EB}$   $-240$  m/s. The magnetic storm was accompanied by a strong negative ionospheric storm. According to the ionosonde st. Pruhonice, Czech Republic ( $50^\circ$  N,  $14.6^\circ$  E) during the main phase of the storm, a significant decrease in  $NmF2$  density by about 60% was recorded, and the height of  $hmF2$  increased by about 40 km compared to the reference day.

The maximum value  $|E_y|$  during the magnetic storm on November 4, 2021, it was  $29$  mV/m, and the plasma transfer velocity  $v_{EB}$  reached almost  $-260$  m/s. The magnetic storm on November 4, 2021 was also accompanied by a negative ionospheric storm, during which there was a decrease in the electron density at the maximum of the F2 layer of the ionosphere and a significant rise

in the height  $hmF2$  – by about 90 km.

The results of a comparative analysis of the experimental data of the st. Pruhonice ionosonde with calculations using the international global model of the ionosphere IRI-2016 and the regional model of the ionosphere CERIM ION, developed at the Institute of Ionosphere, are presented. It is shown that the IRI-2016 model, even with the "F-peak storm model" option, incorrectly reproduces the diurnal variations in both the electron density at the maximum of the F2 layer of the ionosphere and for the height of this maximum  $hmF2$  under disturbed conditions. The regional model CERIM ION, designed for calculating the parameters of the ionosphere in quiet conditions, in comparison with the IRI-2016 model, gives a more reliable forecast of variations in the main parameters of the F2 layer.

In general, taking into account the effects of electric fields during magnetic storms makes it possible to refine, analyze and physically interpret variations in the parameters of dynamic processes in the ionospheric plasma.

**Physics of Nuclei and Elementary Particles**

**Relativistic density functional approach to a unified description of quark-hadron matter**

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The principal element of a unified description of strongly interacting matter within effective theories is the hadronization of quarks at low temperatures and baryonic densities, while the partonic degrees of freedom are being suppressed in this regime. I present a novel approach to attack this problem, which is formulated based on a relativistic density-functional motivated by the string-flip model. Dynamical restoration of chiral symmetry within this approach is ensured by construction of the density functional. The low density/temperature suppression of quark degrees of freedom is provided by increase of the corresponding self-energy already at the mean-field level. I also discuss the connection of the present approach to a Nambu-Jona-Lasinio-type model with density dependent (pseudo-)scalar coupling. Supplemented with the vector repulsion and diquark pairing channels it is applied to model cold quark matter. The corresponding couplings are limited by confronting the results of modeling compact stars with quark cores to the observational data. This allows to construct the mean-field phase diagram of strongly interacting matter. Effects of hadronization of strongly interacting matter are considered as a result of quark correlations beyond the mean field. The correlations caused by (pseudo-)scalar interaction channels are considered within the Gaussian approximation. This explicitly introduces mesonic states into the model. Their contribution to the thermodynamic potential is analyzed within the Beth-Uhlenbeck framework. Due to the different response of the mass spectrum of bound and continuum states to changes of the medium properties the Mott dissociation of mesonic bound states occurs and is interpreted as physical mechanism of the deconfinement transition.

## Physics of Nuclei and Elementary Particles

# Influence of cluster polarization on spectrum and elastic processes in ${}^6\text{Li}$

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The aim of the present report is to study nature of resonance state in  ${}^6\text{Li}$  within an extended three-cluster model. It is well-known that the nucleus  ${}^6\text{Li}$  has two sets of resonance states. The first set is formed by low-energy resonance states which lie close to the  $\alpha+d$  decay threshold and are of positive parity. There are two very narrow and three broad resonance states in the first set. The second set of resonance states consists of high-energy resonance states of negative parity. They are very broad and reside above the  ${}^3\text{H}+{}^3\text{He}$  decay threshold. Different microscopic and semi-microscopic models have been used to study resonance states in  ${}^6\text{Li}$ . As a rule, they have been applied to investigate either low-energy or only high-energy resonance states. In the present report we study both sets of resonance states within one microscopic model. This model was formulated in Ref. [1] and is a three-cluster version of the resonating group method. To study resonance states of  ${}^6\text{Li}$  within a large energy range the model was advanced to take into account two three-cluster configurations  $\alpha+p+n$  and  $t+d+p$ . This allows us to involve in calculations all dominant binary channels, namely,  $\alpha+d$ ,  ${}^5\text{He}+p$ ,  ${}^5\text{Li}+n$  and  ${}^3\text{H}+{}^3\text{He}$ . Besides, these three-cluster configurations also allow us to describe more correctly (adequately) the internal structure of  $d$ ,  ${}^5\text{He}$ ,  ${}^5\text{Li}$ ,  ${}^3\text{He}$  which are represented as a two-cluster configuration  $p+n$ ,  ${}^4\text{He}+n$ ,  ${}^4\text{He}+p$ ,  $d+p$ , respectively.

Calculations of discrete and continuous spectrum states of  ${}^6\text{Li}$  are performed with a nucleon-nucleon potential which was suggested by Tang and coworkers and is known as the Minnesota potential [2]. Parameters of the model and the nucleon-nucleon potential were selected to reproduce the ground state energy of  ${}^6\text{Li}$ . The present model with these parameters fairly good reproduces the energies and widths of the observed resonance states. The dominant decay channels are found for all resonance states. The hierarchy of channels depending on their impact on the energy of the ground and resonance states is established. It is shown that the cluster polarization, associated with the ability of clusters  $d$ ,  ${}^5\text{He}$ ,  ${}^5\text{Li}$ ,  ${}^3\text{He}$  to change their size and shape, plays an important role in formation of the ground state and low- and high-energy resonances in  ${}^6\text{Li}$ .

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**Physics of Nuclei and Elementary Particles**

## **Phase diagram of interacting pion matter and isospin charge fluctuations**

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Equation of state and electric (isospin) charge fluctuations are studied for matter composed of interacting pions. The pion matter is described by self-interacting scalar fields via a  $\phi^4 - \phi^6$  type Lagrangian. The mean-field approximation is used and interaction parameters are fixed by fitting lattice QCD results on the isospin density as a function of the isospin chemical potential at zero temperature. Two scenarios for fixing the model parameters - with and without the first order phase transition are considered, both yielding a satisfactory description of the lattice data. Thermodynamic functions and isospin charge fluctuations are studied and systematically compared for these two scenarios, yielding qualitative differences in the behavior of isospin charge susceptibilities. These differences can be probed by lattice simulations at temperatures  $T < 100\text{~MeV}$ .

## Physics of Nuclei and Elementary Particles

# Constraining baryon annihilation in the hadronic phase of heavy-ion collisions via event-by-event fluctuations

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We point out that the variance of net-baryon distribution normalized by the Skellam distribution baseline,  $\kappa_2[B - \bar{B}]/B + \bar{B}$ , is sensitive to the possible modification of (anti)baryon yields due to  $B\bar{B}$  annihilation in the hadronic phase. The corresponding measurements can thus place stringent limits on the magnitude of the  $B\bar{B}$  annihilation and its inverse reaction. We perform Monte Carlo simulations of the hadronic phase in Pb-Pb collisions at the LHC via the recently developed subensemble sampler + UrQMD afterburner and show that the effect survives in net-proton fluctuations, which are directly accessible experimentally. The available experimental data of the ALICE Collaboration on net-proton fluctuations disfavors a notable suppression of (anti)baryon yields in  $B\bar{B}$  annihilations predicted by the present version of UrQMD if only global baryon conservation is incorporated. On the other hand, the annihilations improve the data description when local baryon conservation is imposed. The two effects can be disentangled by measuring  $\kappa_2[B + \bar{B}]/B + \bar{B}$ , which at the LHC is notably suppressed by annihilations but virtually unaffected by baryon number conservation.

**Physics of Nuclei and Elementary Particles**

# **Critical point and Bose-Einstein condensation in pion matter**

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The Bose-Einstein condensation and the liquid-gas first-order phase transition are studied in the interacting pion matter. Two phenomenological models are used: the mean-field model and the hybrid model. Free model parameters are fixed by fitting the lattice QCD data on the pion Bose condensate density at zero temperature. In spite of some minor differences, the two models demonstrate an identical qualitative and very close quantitative behavior for the thermodynamic functions and electric charge fluctuations. A peculiar property of the considered models is an intersection of the Bose-Einstein condensation line and the line of the first-order phase transition at the critical endpoint.

## Physics of Nuclei and Elementary Particles

# The estimation of pion and kaon maximal emission times in 5.02A TeV collisions at the LHC

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In [1] a simple method allowing one to estimate the times of maximal emission for pions and kaons, created in the LHC Pb+Pb collisions at  $\sqrt{s_{NN}} = 2.76$ -TeV, based on the combined fitting of their  $p_T$  spectra and the dependences of longitudinal femtoscopy radii on the pair transverse mass,  $R_{\text{long}}(m_T)$ , was proposed and tested within the hydrokinetic model (HKM), able to simulate the process of the matter evolution in course of a relativistic heavy-ion collision. The entire evolution process is described as passing in several stages within the model (the initial state formation, the hydrodynamical expansion of continuous medium, the matter particlization, and the final "afterburner" hadron cascade stage). The proposed method was successfully applied to the analysis of the experimental data by the ALICE Collaboration~[2].

In the current work the same method is applied to the femtoscopy analysis of Pb+Pb collisions at a higher LHC energy,  $\sqrt{s_{NN}} = 5.02$ -TeV, within an improved model version - the integrated hydrokinetic model (iHKM), which, in particular, additionally includes the simulation of the pre-thermal stage of the system's evolution and viscous (instead of previously used ideal) hydrodynamics for the description of (quasi)equilibrated expansion of nearly thermalized quark-gluon matter.

The obtained fitting results for pion and kaon maximal emission times in the three centrality classes are consistent with the corresponding approximate time values, estimated based on the model emission function graphs~[3]. Thus, the method can be proposed for use in the experimental analysis of A+A collisions at the current LHC energy. The extracted maximal emission time values decrease, when one goes from central to non-central events. The kaons are emitted later than pions, mainly due to the  $K^*(892)$  resonance decay contribution to the total kaon yield. The  $m_T$  scaling between pions and kaons gets broken because of the strong transverse collective flow at the hydrodynamical stage and the intensive hadron-hadron scatterings at the post-hydrodynamical stage of the collision.

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**Physics of Nuclei and Elementary Particles**

**First results of iHKM at RHIC BES energies: measuring shear viscosity of QGP**

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Integrated hydro-kinetic model was modified and first time applied to baryon-rich matter created in heavy-ion collisions at relatively low energies of RHIC BES program. The model employs a transport approach at the early and late non-equilibrium stages of evolution of the system and viscous hydrodynamics with smooth continuous thermalization in the middle stage of near-equilibrium expansion of quark-gluon plasma. First results for  $p_T$  spectra, elliptic flow, and femtoscopy are presented. Simulations indicate that the most successful description of the existing data corresponds to the lowest possible shear viscosity to entropy density ratio  $\eta/s = 1/4\pi$  and fast thermalization with  $\tau_{th} \sim 0.5\text{fm}/c$ .