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Book of Abstracts

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Morning Session 1

Towards the modeling of impurity migration in a heterogeneous media

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One of the primary tasks of ensuring the safety of objects in contact with polluting objects (for example, radiation waste) is to assess the risks associated with the possible spread of impurities over long distances. Experiments that were carried out on a real natural scale, in which the migration of an impurity injected into a layer including a network of migration channels was studied under natural conditions, showed that in such heterogeneous media, the tracer concentration profiles are significantly asymmetric. In particular, they have an asymmetry strongly shifted towards the flow, in which the decrease in the impurity concentration does not correspond to the classical Fickian law of molecular diffusion and occurs not according to an exponential law, but rather according to a power law [1,2]. Such an anomalous nature of the dispersion of impurities (for example, radionuclides or other polluting components, such as heavy metal atoms) during natural filtration in highly heterogeneous layers is dangerous due to the possibility of their migration over longer distances than follows from estimates made based on of the classical diffusion model.

Models with fractional spatial derivatives used in theoretical works to describe such experiments are, as a rule, limited to the one-dimensional case and are not directly applicable to the calculation of natural processes in three-dimensional anisotropic media. To solve this problem, a concept for using multidimensional stochastic random walk models can be proposed, including modeling Lévy flights in the space of alpha-stable random processes [3].

Alpha-stable random processes are processes characterized by infinitely divisible scenarios (trajectories), which are, in a certain sense, an attractor for all other processes.

If, for example, we consider the well-known Kolmogorov equation [4] as a control equation in the one-dimensional case for different values of the control parameter, then for some certain values of it, it reduces to the usual diffusion equation. At the same time, there is such an interval of numerical values of the control parameter in which it turns into the diffusion equation with fractional derivatives (fractional diffusion equation). And, if the process characterized by the Gaussian distribution describes a random walk of a particle that does not make long (super-diffusive) movements, then under certain conditions we obtain distributions that describe so-called "Lévy flights", which are suitable for modeling the movement of impurities through a system of channels in a given medium (matrix).

In the context described above, for the problems of parameterization of experimental measurement data, this work directly proposes a phenomenological expression for the impurity concentration function, which depends on a small number of parameters and allows the description of the migration process in both classical diffusion and large-scale (super-diffusion) modes.

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Morning Session 1

Towards the influence of compaction on the compressibility of a model bi-component mixture

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There are well-defined indications, following from experimental studies of compressibility (adiabatic compressibility is measured using sound speed measurements, and then isothermal compressibility is restored), to the existence of a dependence of the compressibility of simple bi-component mixtures not only on the molar fractions of the components [1]. It can be assumed that this parameter may be the compaction (packaging) parameter [2].

In this way, this work examines the question of the influence of the packing parameter on the compressibility of a model two-component mixture. For this purpose, it is proposed to use extensions of the model equations of state (for example, the van der Waals equation is chosen) for the case of a two-component mixture together with an equation for compressibility, following from the Carnahan-Starling-Mansoori theory [3], which operates precisely with the compactization factor.

Analytical expressions have been obtained to express the compressibility of a binary mixture through the molar fractions of the components and the compaction of the entire bi-component system. Using the obtained analytical expressions, three-dimensional phase diagrams have been constructed in the axes compressibility, the molar fraction of one of the components, and the compaction of the mixture, allowing one to track the joint influence of these parameters on the equation of state model bi-component system.

As a result of studying the obtained phase diagrams, it was established that the influence of internal parameters (molar composition, compaction) is carried out jointly and consistently (multi-parameter). Mole composition and compaction, for model systems (such as the hard ball model) are among the carefully controlled parameters and thus, the proposed model for describing compressibility is suitable for use to parameterize the results of empirical studies of the dependence of the compressibility of simple binary mixtures (liquid, or granular) to the theoretical description of which the concept of hard spheres is applicable.

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Morning Session 1

How partition function zeros help find out the finite-size scaling above the upper critical dimension

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For many years the question of finite-size scaling above the upper critical dimension dc was a source of many new theoretical results as well as new and interesting works in computer simulations, see [1] for a review . While in the thermodynamic limit system's scaling behaviour is mean-field, for the finitesize systems two scaling regimes are being considered. Simple approach is a trivial renormalization group fixed point, obtained by setting all fields to zero, called Gaussian fixed point, or G-scaling. Second scaling regime introduces a new scaling exponent $q = max(1, d/d_c)$, that governs the scaling of correlation length ξ with system size L, it is called Q-scaling. The latter was confirmed for periodic boundary conditions, both at the infinite system's critical temperature and at the pseudocritical points. For lattices with free boundary conditions the shifting and rounding of the susceptibility peak that occurs at the pseudocritical point are big enough to position the pseudocriticality far from the critical point of the infinite system. This leads to both scaling regimes emerge, so theory predicted G-scaling at T_c and Q-scaling at T_L. Numerical validation of the finite-size scaling for free boundary conditions was not clear, as the boundary effects are too strong to observe the scaling picture accurately. In this work we show the shortcomings of the regular computer simulations methods and improve the quality of the finite-size scaling using the Lee-Yang zeros technique. Using the partition function zeros provides us with the more accurate scaling picture with smaller lattice sizes at hand [2].

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Afternoon Session 1

Theoretical study of a transmon-type qubit connected to a semi-infinite transmission line

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The research is dedicated to a detailed theoretical study of dynamic processes that occur during the interaction of a transmon-type qubit connected to a semi-infinite transmission line with two signals: pump and probe. By manipulating the frequencies and amplitudes of the signals it is possible to explore the system behavior. We use the Lindblad equation formalism to make our calculations. From the solution of the Lindblad equation one can get upper charge level occupation probability as a function of pump and probe signals parameters (amplitudes and frequencies) and build these dependencies.

In Ref. [1] the authors mentioned that the experimentally measured reflection coefficient corresponds to upper charge level occupation probability in the theory. In Ref. [2] the theoretical model describing the system was developed and approved experimentally. The current research is an extension of the corresponding article: here we build the dependencies which were not considered before. Particularly we studied the steady state, by plotting the dependence of upper charge level occupation probability on the probe frequency and the pump frequency. For studying dynamics the upper charge level occupation probability was built as a function of (a) time and the probe frequency; (b) time and the probe frequency. The obtained plots provide a deeper insight into the underlying physical processes and could be valuable for guiding future experiments. Additionally, we address the Lindblad equation using Lindblad superoperators in different bases. In our opinion, this comparative analysis holds significant methodological importance.

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Afternoon Session 1

Optimization of quantum logic gates based on nonadiabatic Landau-Zener-Stückelberg-Majorana transitions

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Quantum logic gates applied to qubits are basic elements of the circuit model used for quantum computations. Usually, quantum gates are realized by a resonant excitation, resulting in Rabi oscillations, which lead to a periodic excitation of the qubit. It has certain limitations and complications, like neglecting counter-rotating terms. We investigate an alternative way for quantum control and performing of quantum logic gates with Landau-Zener-Stückelberg-Majorana (LZSM) transitions [1,2,3] using nonadiabatic driving and alternation of the two stages of evolution: adiabatic evolution and non-adiabatic transitions. We investigate mechanisms, dynamics, and ways to optimize single-qubit LZSM gates [1,3]. We apply the adiabatic-impulse model to describe multiple LZSM transitions [1,3], which we use to create LZSM-based quantum logic gates. Any single-qubit operation can be realized with only two LZSM transitions with an adjustable time of free evolution time before and after those transitions. To gain better fidelity and reduce quantum gates performing time, we can use multiple LZSM transitions. LZSM-based quantum logic gates in comparison with Rabi oscillations based gates allow us to reduce gate time with keeping fidelity high, enabling us to perform more gates before the impact from decoherence and relaxation becomes significant. Fig.1 shows the dynamics for the NOT (X) gate realized by double LZSM transitions.
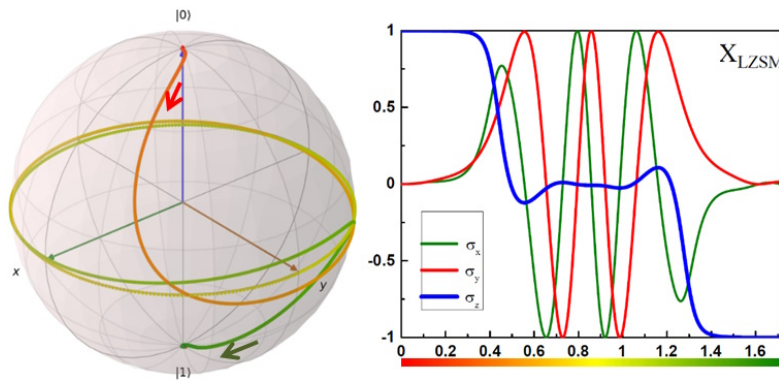
Figure 1: Dynamics for the NOT (X) gate with ground initial state with double LZSM transitions: (a) dynamics on the Bloch sphere, (b) dynamics of Bloch coordinates.

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Afternoon Session 1

Theory of low-frequency electron fluctuations in a quasi-ballistic FET

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Scaling down electronic devices requires studies of physics of nonequilibrium electron transport under highly nonuniform self-consistent electric fields in nanostructures. At that, a relevant theory is a key element of these studies. Here we report theoretical results on physics of nanoscale field effect transistors (FETs), which is a basic device of nanoelectronics. Our main goal was to investigate the electronic processes in a FET channel using shallow water approximations [1] to obtain the analytical expressions for electron and field distributions, as well as electric fluctuations using the Langevin approach [2]. We considered the current-voltage characteristic of the transistor in the stationary mode. For the non-stationary case, we obtained the spatial distributions of the spectral fluctuations density for different parameters of the channel, and the dependence of these values on the stationary parameters We considered two modes of measuring transistor characteristics, with a fixed voltage (A) or current (B), and, correspondingly, suppressed fluctuations of either of these two quantities. In the shallow water approach, the equation of motion for the electrons takes the
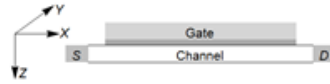

Figure 1: The schematical view of the device we studied

following form:

$$\frac{d\mathbf{n}}{d\xi} = B\frac{\zeta \mathbf{n}^2}{[\zeta^2 - \mathbf{n}^3]}, \; B = \left(\frac{m\varepsilon\varepsilon_0}{e^2 h}\right)^{1/3} \frac{L}{\tau J^{1/3}}, \; \zeta = \frac{j_0}{J}, \; A = \sqrt[3]{\frac{m\varepsilon\varepsilon_0}{e^2 h}} J^{2/3}, \; where \; \mathbf{n} = \frac{n}{A}, \; \xi = \frac{x}{L} \quad (1)$$

Here n is the concentration, L is the channel length, h is the substrate thickness, and m and e are the effective mass and charge. A is a constant, and B is the low-bias resistance of the channel. For the case of Langevin sources $F'(x)$ of fluctuations [2] in the channel, we solve the linearized dynamic equation (2), assuming that the frequency of fluctuations is less than the inverse time of free passage of electrons through the device.

$$\left(\frac{j_0}{n_0} - \frac{e^2 h n_0^2}{m\varepsilon\varepsilon_0 j_0}\right)\frac{du'}{dx} + u'\frac{1}{\tau} - \left[\frac{e^2 h}{m\varepsilon\varepsilon_0} 2\frac{n_0}{j_0} + \frac{j_0}{n_0^2}\right]\frac{dn_0}{dx}u' = F'(x) \quad (2)$$

The noise characteristics are shown on Figs. 2 and 3.
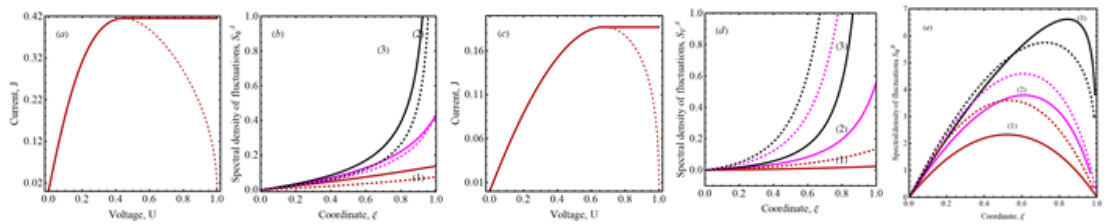
Figure 2: Dimensionless characteristics of quasi-ballistic FETs for $B = 0 : 5$; $Jc = 0 : 415$, panels (a), (b), and $B = 2$, $Jc = 0 : 187$, panels (c), (d). (a), (b): I-V characteristics; current saturation portions are shown conditionally. (c), (d): Spatial distributions of the fluctuations of the velocity and local potential. (e): Local potential distribution in mode B.
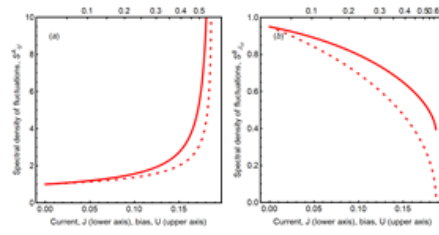
Figure 3: The spectral densities of voltage and current fluctuations in FET (full lines). (a): $S_U^A f$ or the circuit A; (b): S_J^B for the circuit B, for $B = 2$. Dotted lines are relevant estimates with the use of the differential resistance, and the Nyquist formula.

Thus, we were able to obtain the analytical expressions for various stationary and noise characteristics of a FET, solving a non-linear equation system. We used some approximations and a linear approach in the process, in order to solve the dynamic equations in the low-frequency case. We compared our results with the Nyquist formula [2], as well. We discuss contemporary methods of nanoscale measurement of predicted results. These results are available in the preprint [3].

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Afternoon Session 1

Andreev reflection in scanning tunneling spectroscopy of unconventional superconductors

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Motivated by recent experimental observations of unconventional superconductivity in the twisted bilayer and trilayer graphene, we develop a theory of point-contact tunneling into superconductors with arbitrary gap structures and for arbitrary transmission coefficients of the contact. Exploiting the dependence of Andreev reflections on the position of the STM tip relative to lattice symmetry points, we show that the nature of the order parameter can be extracted by combining weak- and strong-tunneling limits of differential conductance. This provides complementary information about the superconducting gap structure beyond the tunneling density of states, strongly facilitating the ability to extract the gap symmetry and its relation to the underlying crystalline lattice. We use the developed theory to discuss recent experimental results on superconductivity in twisted bilayer graphene.

Afternoon Session 1

Long-time asymptotic series for the Painleve II equation: Riemann-Hilbert approach

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We elaborate a systematic way to obtain higher order contributions in the nonlinear steepest descent method for Riemann-Hilbert problem associated with homogeneous Painleve II equation. The problem is reformulated as a matrix factorization problem on two circles and can be solved perturbatively reducing it to finite systems of algebraic linear equations. The method is applied to find explicitly long-time asymptotic behaviour for tau function of Painleve II equation.

Afternoon Session 1

Perturbation equations for Schwarzschild geodesics

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In our work we consider geodesic equations in Schwarzschild space-time with arbitrary external forces and obtain Gaussian perturbation equations for osculating elements in terms of Weierstrass elliptic functions. As an application, we solve the perturbation equations analytically in linear approximation for forces induced by the presence of the cosmological constant in the Schwarzschild-de Sitter metric, which we compared with a known analytical solution. Also, we solve the perturbation equations for hybrid Schwarzschild/post-Newtonian 2.5 order self-forces.

Morning Session 2

Revealing inaccuracies of the GFN1-xTB semi-empirical method with machine-learning toolset

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The change in conformation during biological functioning is a characteristic feature of biomolecules. The presence of various conformers complicates their physics-based modeling, as the properties of each conformer need to be determined separately. Moreover, the relative energies of the conformers become an additional quantity of interest because they determine the probability of each conformation in a real system.

Although ab initio quantum-mechanical methods are the most accurate for determining the physical properties of molecules, their computational costs become prohibitive when applied to biomolecules with a large number of atoms and/or a large number of conformations. Semi-empirical quantum mechanical methods, particularly those based on the tight-binding approximation in density functional theory (DFTB), significantly reduce computational requirements by utilizing parameterized models for the elements of the Fock or Kohn-Sham matrices. However, due to such simplifications, the resulting method can show low accuracy in some cases, despite performing accurately in other cases. In this work, we demonstrate that machine learning (ML) methods such as graph neural networks and ensemble models can be employed to predict errors in determining the relative energies of conformers by the semi-empirical method GFN1-xTB from the DFTB family, based solely on the molecular structural formula as input.

The developed ML ensemble model achieves an accuracy of about 80% in determining whether a given molecule is 'challenging' for GFN1-xTB. This approach can be used to find the molecules that most vividly highlight the shortcomings of the physical model underlying the GFN1-xTB method. We demonstrate that for the 190 molecules selected using the developed model, the average error in relative energies of their conformers obtained by the GFN1-xTB method is 4.2 kcal/mol, in contrast to 1.8 kcal/mol when the same number of test molecules are selected randomly. This indicates that the ML toolset indeed allows for the identification of challenging molecules and can therefore be useful in improving the approximations utilized by semi-empirical methods.

Morning Session 2

The Mutual Influence of Production Rate of Point Defects and Temperature on the Effects of Radiation-Induced Segregation in the Fe-20Cr-8Ni Alloy

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In this paper, a computer simulation of radiation-induced segregation in the Fe-20Cr-8Ni alloy was carried out within the framework of the modified inverse Kirkendall model [1-3]. The dependences of the concentrations of Cr and Ni atoms on the surface of the sample on the rate of production of point defects and temperature, as well as the concentration profiles of Cr and Ni atoms and point defects, were calculated. The influence of the rate of production of point defects and temperature on the concentration profiles of components and point defects is analyzed in detail. It is shown that the effect of the increase in the rate of production of point defects on the concentration profiles of the alloy components can be compensated with a sufficiently high accuracy by a relatively small increase in temperature (Fig.1). This effect is explained by the competition of two mechanisms: (i) increasing the irradiation of the alloy leads to a narrowing of the concentration profiles; (ii) an increase in temperature leads to a broadening of concentration profiles.
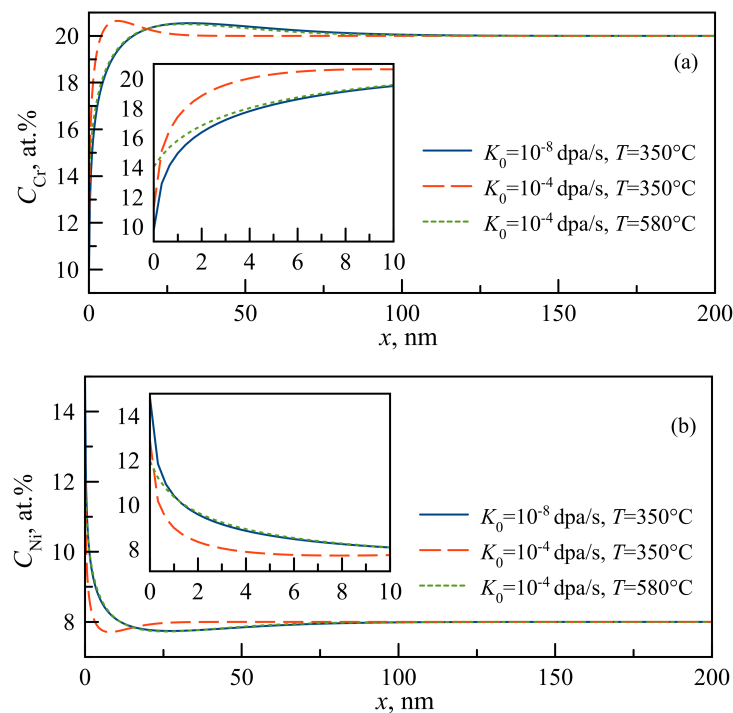
Figure 1: Concentration profiles of Cr and Ni in the Fe-20Cr-8Ni alloy under irradiation.

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Morning Session 2

Spatial coherence of compact sources with respect to X-ray phase contrast imaging formation

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Significant successes and important results of research on synchrotron radiation sources raised a new urgent question, namely the development of bright compact radiation sources with coherence parameters that allow the implementation of phase-informative methods. This is due to the growing demand for the use of new research methods based on X-ray radiation in engineering, materials science and medicine. The study concerns the topical issue of implementation of diffraction research methods on compact radiation sources [1]. Taking into account phase information helps to increase the sensitivity and informativeness of the obtained images, making their use more effective in a wide range of research and diagnostic tasks.

The aim is to determine the research capabilities of various types of installations in solving specific applied problems, as well as to develop applied calculation methods for planning and conducting X-ray phase contrast experiments. X-ray phase contrast arises due to the difference in the phase of X-rays when they pass through objects with different refractive or absorption indices. One of the approaches for modeling X-ray phase contrast is the Fresnel-Kirchhoff scalar diffraction theory [2-4]. This study presents a method for calculating phase-contrast images of test objects. A two-stage algorithm for calculating the X-ray phase contrast image from sources of different shapes and sizes has been developed. The evolution of the wave front along the source-object and object-screen path is taken into account. The source-object and object-screen distances at which it is possible to observe phase-contrast images in the Fresnel region have been found. Simulated images of test objects were obtained in the form of intensity contrast on the screen and its phase profile. As the calculations show, increasing the thickness of certain sections of the test object leads to changes in the phase distribution and intensity of the resulting image. This is manifested in the form of the appearance of intensity maxima at the edges of the object, where there is a fast change in its thickness, as well as minima, where the thickness is the largest, which is explained by a greater deviation of X-rays from their original direction.

The results of the research will be useful for the development of methods for studying the internal structure of materials, as well as for solving problems in medical diagnostics, where X-ray phase contrast can help distinguish tissues with different physical properties, for example, in the study of soft tissues and organs.

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Morning Session 2

Influence of the variable cross section on the domain wall dynamics in curved ferromagnetic nanostripes

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Curvilinear magnetism is an emerging field which connects low-dimensional magnetic architectures with their geometrical properties to describe resulting novel phenomena. Nanoscale curved magnetic stripes are a crucial building block in the race for high-density and ultrafast magnetic memory, and can substantially augment the performance of spintronic devices [1,2]. Here, we aim to theoretically and numerically study how changes in the cross-section area of the curved ferromagnetic nanostripe affect its magnetic structure. Namely, we show that tailoring of the gradient of the cross-section area can be used to control the motion of the domain wall. Although, the magnetic response of the curved nanostripe is already well-studied, in all previous studies cross section of the nanowire was assumed to be constant. Only recently, a new micromagnetic framework emerged that allows the exploration of the changes in the magnetization dynamics caused by the cross-section area gradient [3].

Here, we use the collective variable approach by adapting the q-Φ model to stripes with varying cross section. The description of the domain wall motion in ferromagnetic wires is investigated by considering the temporal evolution of the magnetization vector based on the Landau–Lifshitz–Gilbert equation. To derive the specific equations of motion for the collective variables, the Lagrange-Rayleight formalism is used, where the dependency on the spatial variation of the cross-section area is factored in both the Lagrangian and the dissipative function.

The resulting equations of the domain wall motion are studied for three specific geometries: a straight stripe, an arc of a circle and an Euler spiral. For the case of a straight stripe with absent curvature, we show that the domain wall velocity is mainly determined by the cross-section gradient. For the case of constant curvature, the asymptotic domain wall velocity is shown to have two components: the first component is identical to the speed of the domain wall in the straight wire, while the second one describes the coupling between the curvature and the cross-section gradient. For the case of the wire, whose curvature grows at a constant rate, the asymptotic domain wall velocity has two contributions. The first one is the same as the velocity in the straight wire, however, the second one differs from the previous case and is determined solely by the rate of curvature growth. All analytical predictions are wellconfirmed by the NMAG micromagnetic simulations [4].

The gradient of the cross-section area of the curved ferromagnetic nanostripe creates an internal driving force, which in turn induces the domain wall motion and can explain the recent experimental results [5]. We have shown how the dynamics of the domain wall motion can be modified through tailoring the cross-section area of the nanostripe. Although we showcased our approach only for three specific geometries, it is general and can be applied to a wide class of geometries.

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Afternoon Session 2

Nature of Pauli resonances states in light nuclei

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The resonating group method (RGM) [1] is a rigorous and self-consistent realization of cluster model. It has been numerously proved the RGM is a powerful tool to study the structure of light atomic nuclei and nuclear reactions of different types. Thus it equally well describes bound and continuous spectrum states. The main advantages of the RGM is that it takes into account the internal structure of interacting nuclei (clusters) and correctly treats the Pauli principle. In the standard (initial) version of the RGM, the internal structure of clusters was described by wave functions of the many-particle shell model. Then, many attempts have been made (undertaken) to use more realistic wave functions of clusters. They aimed at a more correct description of interacting clusters and compound system as well. These attempts brought new interesting results. However, they also gave a birth of a new problem, which is called the Pauli resonances and which are considered as a redundant solutions of the RGM equations. It was recognized, the Pauli principle is the origin of the problem.

In our work, we perform a systematic investigation of the Pauli resonance states in the continuum spectrum of light atomic nuclei: ^{6}Li, ^{7}Li, ^{8}Be, ^{9}Be and ^{10}B. These nuclei are considered as two-cluster systems. One of the clusters of two-cluster system, which is weakly bound, is also considered as a two-cluster system. We especially interested in the Pauli resonance states appearing in interaction of neutrons, protons, deuteron, tritons and alpha particles with ^{6}Li. For this purpose, we employ of a microscopic three-cluster model, formulated in [2]. This model uses square-integrable Gaussian and oscillator bases to expand wave function of relative motion of clusters. As a result, the many-particle Schrödinger equation is transformed into a set linear algebraic equations. It is numerously demonstrated that discrete algebraic form of two-cluster Hamiltonian is the best way to analyze effects of the Pauli principle.

It is shown that the Pauli resonance states in selected nuclei lie in the energy range between 11 and 45 MeV, and their widths are varied from 8 keV to 8 MeV. It is demonstrated that in main cases, only one Pauli resonance emerges in continuous spectrum of two-cluster systems. We have also found several cases when two Pauli resonances are formed by interaction of two clusters.

Analysis of wave functions of the Pauli resonance states and the many-particle Schrödinger equation in the discrete space allowed us to formulate an algorithm for elimination of Pauli resonance states. This algorithm suggests new definition of so-called totally-forbidden and almost-forbidden Pauli states which are responsible for creation of the Pauli resonances. It is demonstrated that the suggested algorithm completely eliminates all Pauli resonance states.

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Afternoon Session 2

Bremsstrahlung emission in proton-deuteron scattering and nucleon-nucleon forces

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We will present the results of a study of the bremsstrahlung emission of photons in a process of proton scattering on deuterons. Despite the long history of studies of the interaction of protons with deuterons and the existence of some studies on the subject in such reactions there are some interacting problems that need to be tackled. This stimulates us to develop a new model that allows us to gain more information about processes induced by the $p + d$ interaction and the properties of nuclear forces. Besides, this model is aimed at detailed analysis and interpretation of the existing experimental data on bremsstrahlung emission in these processes. The relative simplicity of the selected nuclei is explained by the fact that it is possible to demonstrate more clearly the effectiveness of the model.

The quantum model of photon emission developed by us is a continuation of the development of methods of bremsstrahlung emission in nuclear processes formulated in [1, 2] (see references therein) with new incorporating ideas of cluster models [3, 4] (see references therein). Within the framework of the model, proton scattering on a deuteron is described as a solution of the quantum-mechanical three-nucleon problem with semi-realistic nucleon-nucleon potentials. This model is applied to study wave functions of continuous spectrum states in the $p + d$ system and then to calculate cross sections of photon emission. Based on this model, a good description of the existing experimental emission data has been achieved [5, 6]. The dependence of the cross sections of bremsstrahlung emission on the shape of the nucleon-nucleon potential is studied in details.

We have applied our method to analyse results of experimental investigations [5, 6] of gamma ray production in $p + d$ interactions. Our analysis revealed that the results of the experiments [5, 6] with chosen parameters (incident energy of proton beam, energy of detected photons) are insensitive to the peculiarities of nuclear forces. However, we have identified another energy region for experiments where it is possible to obtain information about the properties of nuclear forces within the present method with higher accuracy. To make our analysis more complete, we analyze bremsstrahlung properties in a wide range of proton beam energies and photon energies.

Results of our model allow us to predict behavior of bremsstrahlung cross sections which can be used for planning of new experiments. The approach developed can be used to study the bremsstrahlung emission in a large variety of nuclear scattering processes, and also to determine effects of nuclear structure and nucleusnucleus interaction on a such emission.

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Afternoon Session 2

Dynamic Picture of Relativistic Heavy-Ion Collisions

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Collider experiments serve as an unique tool to create and study new forms of strongly interacting matter, such as quark-gluon plasma (QGP). This state of matter is believed to have existed in the microseconds after the Big Bang when temperatures and energy densities were extremely high. However, due to confinement under typical Earth conditions, elementary particles of quantum chromodynamics (QCD) exist only in colorless combinations within hadrons. Lattice QCD calculations show that at zero chemical potential, there is no phase transition between these two states of matter - QGP and hadron gas. However, in baryon-rich regions of the QCD phase diagram, a phase transition of finite order is expected to occur which ends with a critical point.

One of the primary goals of current and future experimental programs, including RHIC BES and CBM, is to search for the signal of the critical point in observables. Such studies demand a comparison with predictions of theoretical models. In this talk, I will present a recently developed integrated Hydro-Kinetic model tailored to describe the full dynamics of the system created in heavy-ion collisions at relatively low energies. Additionally, I will discuss an idea for searching for signals of the critical point through a comparison of model simulations and experimental data.

Afternoon Session 2

Searches for axions in proton-proton and ion-ion collisions at energies of 5.02 TEV and 13 TEV

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As a part of the ATLAS Collaboration experimental measurements of light-by-light scattering in Pb+Pb collisions during 2015 and 2018 at an integrated luminosity of 2.2 nb^{-1} and energy of 5.02 TeV, taking into account the obtained experimental constraints [1], we have modeled the production cross sections of axion production, which is candidate for dark matter with subsequent decay into $\gamma\gamma$. Candidates for light-by-light scattering are selected in events with two photons, pseudorapidity, $|\eta_\gamma| < 2.37$, diphoton invariant mass $m_{\gamma\gamma} = 5 - 30$ GeV, and an interaction constant of the order of 10^{-3} GeV^{-1} [2]. The obtained calculations showed the dependence of the cross section on the number of axion events (Fig. 1), on the energy in the center of mass system (Fig. 2), and on the mass distribution of axions.
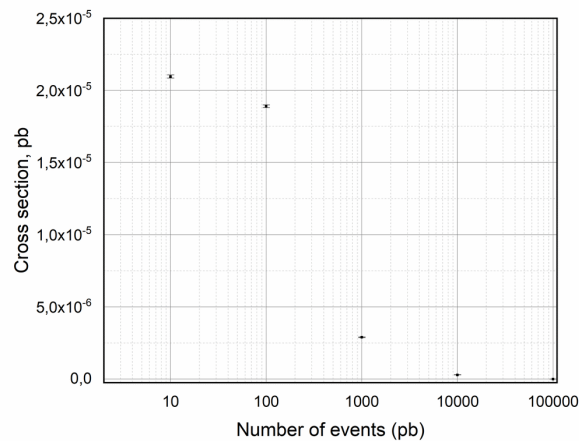

Figure 1: Dependence of the axion cross-section on the number of axion events (based on Monte Carlo simulations in SuperChic v.4.2).
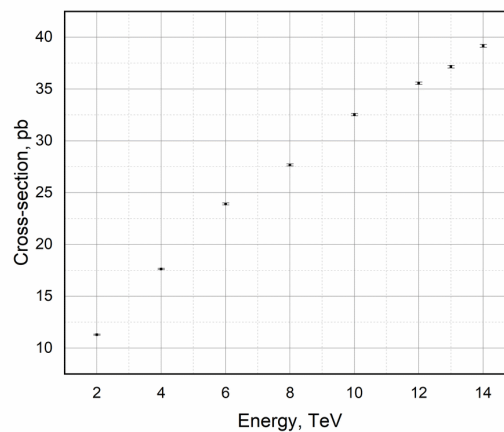

Figure 2: Dependence of the axion cross section at different beam energies at the center of mass system.

Proton-proton and ion-ion collisions were processed for QCD-axion formation using the SuperChic v.4.2 Monte Carlo event generator [3]. Corresponding production cross sections were obtained and compared with recent measurements of light-by-light scattering by ATLAS and CMS collaborations at the LHC during lead-to-lead collisions [4,5]. It is shown that the axion production cross section in proton-proton collisions is seven orders of magnitude larger than that in Pb+Pb collisions at an energy in the center-of-mass system of 5.02 TeV. An order of magnitude difference in the axion production cross section in proton-proton collisions for single dissociation in relation to double dissociation at an energy of 5.02 TeV and a mass range of 5-30 GeV was revealed (approximately 20-21 pb to 9-10 pb, depending on the model). In the same mass range, the axion production cross sections were calculated at 13 TeV and a difference of about 2.5 times in the axion production cross sections for single dissociation versus double dissociation was found. The advantage of the 2nd model at 5.02 TeV and the 1st model at 13 TeV was found. The results of calculations for the four models are presented in Table 1.

E, TeV	Cross section for each model (pb)							
	1		2		3		4	
	Single dis.	Double dis.	Single dis.	Double dis.	Single dis.	Double dis.	Single dis.	Double dis.
5,02	20.908 ± 0.081	9.167 ± 0.079	20.926 ± 0.081	9.219 ± 0.079	20.922 ± 0.081	9.161 ± 0.079	20.905 ± 0.081	9.086 ± 0.079
13	$0.461 \times 10^{-4} \pm 0.31 \times 10^{-6}$	$0.176 \times 10^{-4} \pm 0.18 \times 10^{-6}$	$0.461 \times 10^{-4} \pm 0.31 \times 10^{-6}$	$0.171 \times 10^{-4} \pm 0.165 \times 10^{-6}$	$0.416 \times 10^{-4} \pm 0.26 \times 10^{-6}$	$0.173 \times 10^{-4} \pm 0.183 \times 10^{-6}$	$0.419 \times 10^{-4} \pm 0.27 \times 10^{-6}$	$0.173 \times 10^{-4} \pm 0.183 \times 10^{-6}$

Figure 3: Table 1: The axion production cross-sections in the 5-30 GeV mass region for 4 models.

The analysis of experimental data with 441 candidates for axions obtained during proton-proton collisions at an energy of 13 TeV [6] led to the need for us to search for a narrow resonance in the distribution of diphoton masses in the mass range of 5−1400 GeV with the number of events of 100,000. The obtained data do not exceed the experimental value of the upper limit of the production cross-section of a narrow resonance and are about 0.024 fb.

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Afternoon Session 2

Contribution of one-loop corrections in the decoupling limit of generalized Yukawa model

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There exist many models of physics beyond the Standard model (SM) which introduce new heavy particles. Signals of such new states could be parametrized either within a complete model of new physics or its low-energy approximation. The latter consists of effective Lagrangian (EL), which describes effects of interactions with heavy particles on the dynamics of light fields when heavy states decouple. Parameters of this EL should be constrained in experimental data analysis. These constraints, in turn, are translated into limits on parameters of a corresponding complete model. This approach is employed in many researches. In our investigation we show that the EL considered in this treatment is valid only if loop corrections coming from the light sector of a corresponding complete model are negligible in the decoupling limit.

Our research is conducted for two scattering processes which take place in s- and t-channel, respectively. Transformational properties of fields and complex interactions within the SM are inessential for our analyzis. Hence, we consider generalized Yukawa model instead of a complete SM extended with some new states. We begin with the following Lagrangian of a complete model:

$$\mathcal{L} = \frac{1}{2}\left(\partial_\mu \phi\right)^2 - \frac{1}{2}\mu^2\phi^2 + \frac{1}{2}\left(\partial_\mu \chi\right)^2 - \frac{1}{2}\Lambda^2\chi^2 - \lambda\phi^4 - \rho\phi^2\chi^2 - \xi\chi^4 + + \sum_{a=1;2} \bar{\psi}_a\left(i\hat{\partial} - m_a - g_\phi\phi - g_\chi\chi\right)\psi_a$$

(1)

This model consists of two scalar fields ϕ and χ and two fermionic fields ψ_1 and ψ_2. We put χ boson to be much heavier than the other particles of the model, so $\Lambda \gg \mu$; m_1; m_2. We derived the following low-energy EL for this model in the limit when χ boson decouples:

$$\mathcal{L}_{eff} = \frac{1}{2}\left(\partial_\mu \phi\right)^2 - \frac{1}{2}\mu^2\phi^2 - \lambda\phi^4 + \sum_{a=1;2} \bar{\psi}_a\left(i\hat{\partial} - m_a - g_\phi\phi\right)\psi_a + \frac{g_\chi^2}{2\Lambda^2}\left(\bar{\psi}_1\psi_1 + \bar{\psi}_2\psi_2\right)^2.$$ (2)

Here the last term describes effective four-fermion interactions which approximate contributions of the heavy scalar in observables when χ decouples. The other terms in (2) describe dynamics of the model light sector if $g_\chi = 0$.

Two scattering processes were considered within the complete model (1) and EFT (2) - these are $\psi_1\bar{\psi}_1 \to \psi_2\bar{\psi}_2$ and $\psi_1\psi_2 \to \psi_1\psi_2$. Cross-sections of these processes were derived within the complete model (1) in the improved Born approximation and within the EFT (2). Contributions of radiative corrections into the cross-sections of these processes were estimated in the decoupling limit. We investigated scenarios where χ boson has a mass in the interval $20\mu \le \Lambda \le 200\mu$.
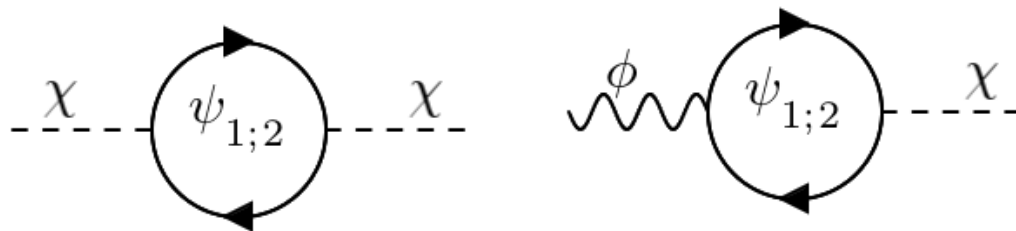
(a) Loop corrections to the ϕ boson mass

(b) Diagram of one-loop mixing of light and heavy scalars of the model

Figure 1: One-loop diagrams which become significant at low energies for some values of the model coupling.

We found out that if $|g_\phi|$ and $|g_\chi|$ are small, then the loop corrections are negligible and the EL (2) is applicable for description of the scattering processes at low energies. For the values of m_1, m_2 and μ chosen in our research this takes place if $|g_\phi| < 0.4$ and $|g_\chi| < 0.4$.

If $|g_\chi|$ is big, then loop corrections to χ boson mass are considerable even at low energies. In our model, we have that if $|g_\chi| > 2.5$ then corrections displayed in Fig. 1a have a magnitude of more than $10\,\%$ of the χ boson mass. These corrections suppress the contribution of the heavy scalar in a reaction cross-section. Hence, if $|g_\chi|$ is big, then (2) significantly overestimates χ boson contribution in a cross-section when χ decouples.

If $|g_\phi|$ is not small, then contribution of the scalar fields one-loop mixing is significant in both s- and t-channels. One-loop mixing of ϕ and χ is introduced by the diagram in Fig. 1b. In our model, we get that if $|g_\phi| > 1.5$, then modulus of the contribution of scalars one-loop mixing in the matrix elements of the considered reactions is bigger than $50\,\%$ of the four-fermion interaction term modulus at $s \gtrsim \mu^2$ and $|t| \gtrsim \mu^2$. This was observed in the limit when loop correction in Fig. 1a is negligible. To conclude, in our research we have derived the conditions when radiative corrections to interactions with the heavy boson are negligible in the decoupling limit in cross-sections of reactions within the generalized Yukawa model. According to these conditions, radiative corrections become significant if the interactions between light fermions and either light or decoupled scalar are not feeble. In such scenarios, expression (2) should not be used as the low-energy approximation of the model (1). The results obtained in this investigation could be applied to some models of new physics which extend the SM, such as the two-Higgs-doublet model (2HDM). The latter has a limit when new heavy particles decouple. So, low-energy EL exists for it. Contributions of radiative corrections into cross-sections within the 2HDM should be estimated in the limit when heavy fields beyond the SM decouple. This is the problem left for the future.

Afternoon Session 2

Constraints on the parameters of the neutrino extension of the Standard Model

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This work examines limitations on the neutrino extension parameters of the Standard Model of elementary particle physics. A simple relationship between the observed quantities, elements of the matrices S and R was obtained, which is valid for non-zero masses of active neutrinos and for different values of masses of heavy sterile neutrinos. Experimental constraints on the elements of the S and R matrices were improved, and constraints on U_{tot}^2 depending on the mass of a heavy neutrino with right chirality were obtained. The expression for the baryon asymmetry of the early Universe also was analyzed.

Afternoon Session 2

Quantum van der Waals theory of nuclear matter with quarkyonic phase

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We extend the Quantum van der Waals description of isospin symmetric nuclear matter at zero temperature to a high baryon density region by incorporating the continuous transition to quark matter in accordance with the recently proposed quarkyonic approach. The resulting equation of state exhibits the nuclear liquid-gas transition at $n_B \leq \rho_0$ and undergoes a transition to quarkyonic matter at densities $n_B \approx 1.5 - 2\rho_0$ that are reachable in intermediate energy heavy-ion collisions. The transition is accompanied by a peak in the sound velocity. The results depend only mildly on the chosen excluded volume mechanism but do require the introduction of an infrared regulator Λ to avoid an acausal sound velocity. We also consider the recently proposed baryquark matter scenario for the realization of the Pauli exclusion principle, which yields a similar equation of state and turns out to be energetically favored in all the considered setups.

Afternoon Session 2

Molecular dynamics analysis of particle number fluctuations of a first-order phase transition

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We study the critical point effects on particle number fluctuations both in the crossover ($T > T_c$) and mixed phase ($T < T_c$) regions by means of molecular dynamics simulations of a Lennard-Jones fluid, motivated by the ongoing search for the QCD critical point in heavy-ion collisions.

In the crossover region, we find large fluctuations associated with the critical point in coordinate space, but in the absence of collective flow and expansion, they are essentially washed out when momentum cuts are imposed instead.

In the mixed phase region, the behavior depends on whether the system is in a metastable nucleation or cavitation region, or in the spinodal decomposition region, and can be interpreted in terms of simplified analytic models. For the case of nucleation, we find that fluctuations are qualitatively described by a non-interacting cluster model.

The spinodal decomposition, on the other hand, leads to large fluctuations in coordinate space, which can be understood to arise due to the interplay between the size of the acceptance region and that of the liquid phase.