# XIII Conference of Young Scientists "Problems of Theoretical Physics"

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## **Book of Abstracts**

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## Does quark-gluon plasma form in proton-proton collisions?

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In relativistic heavy-ion collisions a hot and dense thermalized matter of deconfined partons, the Quark-Gluon Plasma (QGP), is created. Its global properties can be characterized by the measurements of particles in the low transverse momentum (or "soft") regime, which represents over 95% of created particles. Many soft observables in proton-proton (pp) collisions at the highest LHC energies exhibit similar behavior as in heavy-ion collisions. Such observables can be interpreted as signals of QGP in pp collisions. We will review some of them in this talk.

The recent experimental results on Bose-Einstein correlations (BEC) of like-sign charged pions yield some new interesting results. Both ATLAS and CMS collaborations measured the source radius  $R_{HBT}$  and particle correlation strength  $\lambda$  as a function of charged particle multiplicity  $N_{ch}$  (up to 300). Discovered source size saturation at high multiplicities  $N_{ch} > 100$  along with low values of  $\lambda$  are not typical for heavy-ion collisions. Thereby these results call into question the formation of QGP in pp experiments.

In this talk we will discuss a simple analytic model of an ideal gas of identical bosons that can quantitatively reproduce HBT data. We claim that the peculiarities of discussed experimental results might be observed from a completely thermal system if one considers subensembles of fixed but high enough multiplicities with noticeable Bose condensation. In the proposed model increase in particle multiplicity, enhances the ground-state contribution to particle momentum spectra and leads to the suppression of the Bose-Einstein momentum correlations.

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# Critical point particle number fluctuations from molecular dynamics

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We study fluctuations of particle number in the presence of a critical point by utilizing molecular dynamics simulations of the classical Lennard-Jones fluid in a periodic box. The numerical solution of the N-body problem naturally incorporates all correlations, exact conservation laws, and finite size effects, allowing us to study the fluctuation signatures of the critical point in a dynamical setup. We find that large fluctuations associated with the critical point are observed when measurements are performed in coordinate subspace, but, in the absence of collective flow and expansion, are essentially washed out when momentum cuts are imposed instead.

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# Two methods for computation of the sensitivity region of the intensity frontier experiments

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The standard model is a remarkably consistent and complete quantum field theory. However, it fails to explain some fundamental problems such as the baryon asymmetry of the Universe, dark matter, and neutrino oscillations. Therefore SM is incomplete and requires an extension.

One possible approach is by adding new particles to the theory. There are two possible answers to the question "Why do we not observe particles of new physics in experiments?" The first answer is the following. The new particles are very heavy and can not be produced in modern accelerators like LHC. To detect them one has to build more powerful and more expensive accelerators. There is another possibility. The particles of new physics can be light particles that feebly interact with SM particles. The last case is very interesting for the experimental search of the new physics in the intensity frontier experiments just now. There are different choices of new renormalized interaction Lagrangian of particles of new physics with SM particles. It's called portals.

In order to detect them a lot of experiments were suggested. To know which one is best and relevant, a sensitivity region is built. This task is not trivial and may take a lot of time, so the question of the fastest and most precise method is crucial.

In this paper, we compare two approaches to computing the sensitivity region of the intensity frontier experiments. Namely, the analytical and Monte-Carlo based approach. We do it by computing the sensitivity region of the SHiP experiment for the detection of a GeV-scale singlet neutral scalar, produced in decays of B mesons [1,2].

We decided to look at the scalar portal on the one hand due to the relative simplicity of this model. Monte-Carlo methods and analytical approach were implemented using Wolfram packages. Some calculations regarding data lists were done in C++.

Our analysis shows that both methods give approximately the same result, but take different times to compute. We conclude that in a case where the probability distribution function of the initial mesons is given in an analytical form, the analytical approach takes less time and is more suitable. If the distribution is given by a data list, Monte-Carlo method is more suitable and more accurate, but the analytical method allows us a faster estimate of the sensitivity region with a smaller, but good enough accuracy.

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## On Landauer-Büttiker formalism from a quantum quench

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We study transport in the free fermionic one-dimensional systems subjected to arbitrary local potentials. The bias needed for the transport is modeled by the initial highly non-equilibrium distribution where only half of the system is populated. Additionally to that, the local potential is also suddenly changed when the transport starts. For such a quench protocol we compute the Full Counting Statistics (FCS) of the number of particles in the initially empty part. In the thermodynamic limit, the FCS can be expressed via the Fredholm determinant with the kernel depending on the scattering data and Jost solutions of the pre-quench and the post-quench potentials. We discuss the large-time asymptotic behavior of the obtained determinant and observe that if two or more bound states are present in the spectrum of the post-quench potential the information about the initial state manifests itself in the persistent oscillations of the FCS. On the contrary, when there are no bound states the asymptotic behavior of the FCS is determined solely by the scattering data of the post-quench potential, which for the current (the first moment) is given by the Landauer–Buttiker formalism. The information about the initial state can be observed only in the transient dynamics.

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## / Book of Abstracts

## Morning session

## Evidence for the galactic neutrino emission

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The high-energy gamma-ray observations presume that the galactic emission is dominated by pion decay flux from cosmic ray interactions in the interstellar medium, with moderate contribution from isolated sources. In some isolated sources, gamma-rays may also be produced by the hadronic process, which implies the neutrino emission. However, no multi-messenger neutrino+gamma signal from the galactic sources were observed so far.

We present the first evidence for the isolated galactic source neutrino emission in the IceCube 10 year public data, as well as the new results for the galactic diffuse emission using the full archival dataset of the Antares neutrino observatory.

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## Hybrid stars and the properties of the special point

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We study hybrid stars containing the color superconducting quark matter phase in their cores, described by the relativistic density functional approach. The hadronic matter was modeled within the realistic DD2 equation of state (EoS). We show that depending on the dimensionless vector and diquark couplings of quark matter characteristics of the deconfinement phase transition are varied, allowing us to study the relation between those characteristics and mass-radius relation of neutron stars with quark cores. Moreover, we show that the quark matter EoS can be fitted by the constant speed of sound parameterization giving a simple functional dependence between the most important parameters of the EoS and microscopic parameters of the initial Lagrangian. Based on it, we analyze the properties of the special point of the neutron star sequences.

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## Heating due to a spin-down compression in hybrid stars

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The spin-down of a compact star causes perturbations in the internal chemical equilibrium state, and, consequently internal heating dubbed as rotochemical heating. Moreover, the fact that the cores of compact stars are thought to reach baryon densities as high as a few times the nuclear saturation density, renders them ideal candidates of being host to deconfined quark matter, the latter implying the existence of hypothetical objects such as hybrid stars and quark stars. We study the effect of this heating mechanism on the thermal evolution of millisecond pulsars with quark core, considering that both phases, i.e. hadron and quark matter, departured from beta equilibrium. The main emphasis is given to the impact of deconfinement phase transition on the rotochemical heating.

# Quantum impurity simulator operating in the fractional quantum Hall regime

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It is well-known that a single-electron transistor (SET) device provides a perfect playground for simulating various quantum impurity models, a class of systems defined by the finite number of local degrees of freedom coupled to one or few bath continua. This is due to the Coulomb blockade phenomenon that is the origin of the charge quantization in the quantum dot (QD). Recently, the charge implementation of the multi-channel Kondo model has been achieved in breakthrough series of experiments [1, 2]. The device in [1,2] has been designed in a hybrid metal-semiconductor SET formed in a two-dimensional electron gas, where the QD is connected to few reservoirs via nearly open single-mode quantum point contacts (QPC). In contrast with the original spin-1/2 impurity problem, where Kondo effect is attributed with the spin degree of freedom, the quantum pseudo-spin in the charge Kondo implementation is represented by two degenerate macroscopic charge states of the QD [3,4]. Together with the high tunability of the one-dimensional (1D) conducting channels entering the QD, this provides access to the study of the multi-channel Kondo physics.

In this talk, I will discuss how electron-electron interactions in 1D conducting channels in the presented above device affect the Kondo physics. To cover effects of interaction, I utilize the Luttinger-liquid model. In real experiment [1,2], effects of Luttinger-liquid may be observed if the hybrid metal-semiconductor SET device will operate in the fractional quantum Hall regime with filling factor  $\nu=1/m$ , where m is odd integer. In case of two-terminal SET, when the problem is mapped onto the 2-channel charge Kondo model, I predict that the power of leading temperature correction to the conductance is determined by the fractional filling factor. In case of the multi-terminal setup, the SET device can be treated as the simulator of the Luttinger-liquid with an impurity, whose effective interaction parameter is determined by the filling factor  $\nu$  and number of open ballistic channels. I will discuss the conductance scaling in the weak and strong tunnel regimes in order to characterize the low temperature transport behavior of the multi-channel charge Kondo circuits.

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## Convective thermomagnetic effect in normal and superfluid systems

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It is known that the motion of a medium results in an interaction between the electric and magnetic fields [1]. In particular, the motion of a dielectric in an external magnetic field  ${\bf H}$  will lead to its polarization. It is generally assumed that the speed of motion is determined by the mechanical motion of the system. There are, however, situations where this motion is associated with a temperature gradient  $\nabla T$ .

One of them is related to counterflow thermal conductivity (often referred to as superthermal conductivity) in superfluid systems, due to which even small temperature gradients ( $\nabla T \approx 10^{-3} K$ ) lead to significant fluxes of the superfluid and normal components in the absence of an average mass flux. As shown in [2, 3], in the presence of an external magnetic field, these flows lead to a polarization of the liquid and the appearance of electric fields in the surrounding space, which can be observed by modern experimental methods.

Another situation is the development of thermogravitational convective instability in normal systems, which consists in the mechanical disequilibrium of a hydrodynamic system under the action of a temperature gradient. As a result, in the presence of a magnetic field the system also acquires polarization, which, in turn, can lead to the appearance of an electric field in the surrounding space. The measurement of this field can be used as a basis for creating a sensitive device for determining temperature gradients.

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# Anomalous electromagnetic field reflection and transmission in Weyl and Dirac semimetals

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The current response to an electromagnetic field in a Weyl or Dirac semimetal becomes nonlocal due to the chiral anomaly activated by an applied magnetic field. The nonlocality develops under the conditions of the normal skin effect and is related to the valley charge imbalance generated by the joint effect of the electric field of the impinging wave and the static magnetic field. The length scale for the nonlocality is determined by the diffusion length of the valley charge imbalance, which does not violate the local electric charge neutrality. It is predicted that the signatures of this nonlocality can be found in the transmission and reflection of electromagnetic waves. In view of a weaker decay of the anomalous components of the electric field in the nonlocal regime, it is possible to achieve an enhancement of the electromagnetic wave penetration depth. For reflected electromagnetic waves, the chiral anomaly leads to a decrease of the dissipative part of the surface impedance with the magnetic field; these anomalous effects are reduced in the nonlocal regime.

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# Multiscale hybrid model of liquids: modified equations of motion

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Co-authors: Dmitry Nerukh 2; Vitaliy Bardyk 3

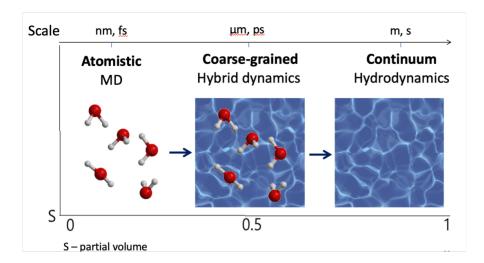
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Classical Molecular Dynamics (MD) methods are the most accurate simulation methods. Solving Newtonian equations of motion by computing the inter-particle forces provides detailed information about the system at the atomistic scale. Nowadays these methods could be used for obtaining a representation of some macroscopic (thermodynamic) and some microscopic (as radial distribution functions and autocorrelation functions) properties of some liquids, qualitative or quantitative descriptions of complex biomolecular structures and their functionality.

Modern specialized computers can simulate liquid molecular systems of several hundred million atoms in size (tens of nanometers across) using classical molecular dynamics (MD) methodology. However, modelling of processes at biologically relevant times (microseconds to milliseconds) is likely to remain infeasible in the framework of existing computational molecular dynamics concepts (at most hundreds of picoseconds - few nanoseconds can be achieved now. One of the approaches that make it possible to implement modelling on a larger scale - is MD-continuum coupling, in which the modelling of part of the MD-region is replaced by continuum representation. But the coupling of MD and HD models is a challenging task.

Different techniques are applied to match MD behaviour to continuum evolution and a range of constraint algorithms has been developed for coupling. Our Multiscale hybrid model of liquids is based on the method, proposed by Smith ER [1], where he used the Gaussian principle of least action to obtain the equations of motion of particles in the extreme case when the correspondence of the pulse MD and HD is ensured.



In order to obtain a generalized equation of motion for the MD-HD coupling scheme so as to obtain the classical equations for MD and HD in extreme cases, and to ensure a smooth transition from no representation to another in intermediate cases, the liquid system has been described as "two-phased" mixture. The two phases are a Lagrangian and an Eulerian representation of the same chemical substance, which correspond to the atomistic (MD) and the continuum (HD) model, respectively. The partial concentration of each phase is determined by parameter s. The MD phase and the HD phase concentration correspond to s and 1- s, respectively ( $0 \le s \le 1$ ). In general, s is a user-defined scale function of space and time, which controls how much atomistic information is required in a

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particular region of the simulation domain. Control Volume formulation can be used to build a strict link between discrete and continuous representations.

For the coupling of MD and HD, the momentum in the hybrid region is adjusted to be the same as the MD. This is done by applying a constraint force to the molecular equations of motion. The method to constrain the momentum in a control volume is derived using both the Principle of Least Action and Gauss's principle. Constrained equations of motion have been derived, using constrained Lagrangian and it has been shown, that equations of motion obtained from Gauss's principle of least constraint and Gauss's principle are identical, so the Principle of Least Action is physically sound in this case.

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## Collective water vibrations in a DNA hydration shell

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In aqueous salt solutions, DNA structure adopts a double-helical shape due to the interactions with water molecules and metal ions around the macromolecule. The ion-hydration shell stabilizes the double helix and may be considered as an integral part of the DNA structure. In the present work, the collective dynamics of DNA hydration shell is studied using classical all-atom molecular dynamics approaches. The spectra of vibrational density of states (VDOS) for water molecules around DNA double helix have been analyzed in details. The results have shown that VDOS spectra of the DNA hydration shell may be approximated by 6 vibrational modes in the range from 30 cm $^{-1}$  to 300 cm<sup>-1</sup>. The modes demonstrate significant differences in the collective vibrational dynamics of water molecules in the DNA hydration shell, compared to the bulk water. This deviation occurs due to enhanced non-bonded interactions of DNA atomic groups with water molecules constraining their mobility. In particular, our calculations have shown the complete damping of symmetrical stretching vibrations of hydrogen bonds between water molecules (the mode near 160 cm<sup>-1</sup>), being present in the bulk. Such detailed atomistic analysis of water collective motions has been applied to DNA systems for the first time. This can provide a qualitative interpretation of the potential experimental data on DNA solutions. The foregoing results can shed light on fundamental processes of DNA function in a living cell, particularly, indirect protein-nucleic recognition.

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## Pulsed Electrical Field Impact on Cyanide Biodegradation by Pseudomonas fluorescens

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The impact of the pulsed electrical field on the cyanide biodegradation process

was investigated in this work. In the experiment, *Pseudomonas fluorescens* bacteria was treated by the pulsed electrical field for 15 mins ( $f = \sim 100 \sim \text{Hz}$ , impulse duration is 1 ms) before adding to the solution with Na[Ag(CN)<sub>2</sub>] complex, and the appropriate kinetics was described [1]. During the cyanide biodegradation process, cyanide blocks the respiratory centers (RCs) of bacteria, but simultaneously bacteria degrade cyanide using the respiratory mechanism [2]. Theoretical analysis of the cyanide biodegradation kinetics was carried out in [3].

The purpose of this work is to introduce a phenomenological model (1-2) that explains the cyanide biodegradation process in [1], and to describe the impact of pulsed electrical field on respiratory parameters of bacteria.

$$\frac{dn}{dt} = -(\gamma_0 + \gamma_1 C) n + (g_0 + g_1 n) (1 - n) - a (1 - C)$$
(1)

$$\frac{dC}{dt} = -\alpha n \frac{C}{C + C_m} \tag{2}$$

where n is a relative number of active RCs that can degrade cyanide, C is a cyanide concentration in the solution,  $\gamma\left(C\right)=\gamma_0+\gamma_1C$  is the rate of RC deactivation for low cyanide concentrations,  $\gamma_0$  and  $\gamma_1$  are constants.  $g\left(n\right)=g_0+g_1n$  is the rate of RC activation,  $g_0$  and  $g_1$  are constants.  $\alpha$  is the maximum rate of the cyanide destruction,  $C_m$  is the Michaelis constant, a is the rate of RCs deactivation caused by-product generation in the solution. Note that the system (1-2) is already normalized.

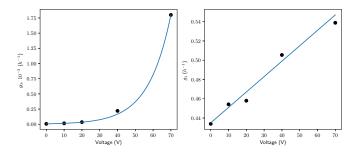


Figure 1: Dependencies of the system parameters on the voltage of pulsed electrical field.

During the analysis of the dependence of absorbed oxygen on cyanide concentration from [4], we identified the following relations:

$$\alpha/C_m = g_1 + g_0/D^2 - \frac{\gamma_1}{AB}$$
 (3)

and

$$C_m = \frac{2}{B} \left( g_1 + g_0 / D^2 - \frac{\gamma_1}{AB} \right) / \left( 2 \frac{\gamma_1}{AB} - 2 \frac{g_0 A}{D^3} - g_1 - \frac{g_0}{D^2} \right), \tag{4}$$

where A, B and D are constants. Thus parameters responsible for the rate of cyanide biodegradation are dependent on the parameters related to the respiratory activity of bacteria. In addition, we found

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that  $\gamma_0 = g_1 - g_1 D - g_0 + g_0/D$ . For other parameters, we identified the dependencies on the voltage of the pulsed electrical field (Fig 1).  $g_1$  and  $\gamma_1$  have linear dependence on voltage. Parameter a is not dependent on voltage. Also, we applied the aforementioned model and results to the cyanide biodegradation experiment in [4] after the re-normalization.

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## Phase transitions in a system of self-interacting particle-antiparticle

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The thermodynamic properties of a particles and antiparticles boson system with a strong interaction at finite temperatures are studied within the framework of the thermodynamically consistent Skyrme-like mean-field model. The mean field contains both attractive and repulsive terms. Isospin density is conserved for all temperatures. Self-consistency relations between the mean field and thermodynamic functions are derived. It is shown that, when attractive mean field is lesser than the critical value  $A_c$ , only one component undergoes the phase transition of second order to the Bose-Einstein condensate at the critical temperature  $T_c$ . For sufficiently strong attractive interactions when  $A>A_c$  the meson system develops a 1st order phase transition at temperature  $T_{cd}$  via forming a Bose condensate and releasing the latent heat. In this case both components develop Bose-Einstein condensate which is characterized by a constant total density of particles. At the point where a curve of particle density touches a critical curve  $(A=A_c)$ , there exists a point-like or virtual phase transition of the 2nd order, i.e., a phase transition without setting the order parameter.

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