

Poster session
Programme Advisory Committee
for Condensed Matter Physics
(28 June, 2021)

Poster abstract	Remarks
<p>1. Effect of charged lipids on β-amyloid peptide interactions with a phospholipid membrane</p> <p style="text-align: center;">A. Ayriyan^{1,2}, D. Badreeva^{1,3}, N. Kučerka^{4,5}</p> <p>¹<i>Meshcheryakov Laboratory of Information Technologies, JINR, Dubna, Russia</i> ²<i>A.I. Alikhanyan National Science Laboratory, Yerevan, Armenia</i> ³<i>Dubna State University, Dubna, Russia</i> ⁴<i>Frank Laboratory of Neutron Physics, JINR, Dubna, Russia</i> ⁵<i>Faculty of Pharmacy, Comenius University, Bratislava, Slovakia</i></p> <p style="text-align: center;">dinkulenok@yandex.ru</p> <p>Alzheimer's disease is a conformational disease caused by the formation of senile plaques consisting primarily of Amyloid-beta peptides. Amyloid-beta (β-amyloid) is a peptide, whose physiological role is not fully known. The crucial role in the process of Aβ accumulation is likely imparted by peptide-membrane interactions. Theoretical studies were carried out for better understanding of physicochemical processes taking place in biomembranes. The theoretical study involved molecular dynamics simulations of the anionic (DMPC + DMPS) membrane interaction with Amyloid-beta 25-35 peptide. Basic parameters, such as radial distribution functions, bilayer thickness and order parameter, were determined. It was shown that the presence of anionic lipids had an effect on the Aβ peptide-lipid interactions. The preferred location of the peptide was also determined. This work was carried out under support of the Russian Science Foundation grant 19-72-20186.</p>	
<p>2. High-performance analysis of the nucleus-nucleus elastic scattering data within the microscopic model of optical potential: scattering of $^{12,14}\text{Be}+^{12}\text{C}$ at 56 MeV/nucleon</p> <p style="text-align: center;">M.V. Bashashin^{1,2}, M.B. Kakenov¹, E.V. Zemlyanaya^{1,2}</p> <p>¹<i>Meshcheryakov Laboratory of Information Technologies, JINR, Dubna, Russia</i> ²<i>Dubna State University, Dubna, Russia</i></p> <p style="text-align: center;">bashashinmv@jinr.ru</p> <p>The MPI/C++ /Fortran package of computer codes has been developed for the high-performance numerical analysis of experimental data on nucleus-nucleus elastic scattering within a microscopic model of the optical potential (OP). In the package, a modified DWUCK4 Fortran-code for calculating the physical characteristics of elastic scattering based on the numerical solution of the corresponding Schrödinger equation has been incorporated into the C++ framework, which is responsible for the input-output procedure and the comparison of numerical results with experimental data. MPI-based parallelism allows one to efficiently calculate observables depending on the depths of real and imaginary parts of the microscopic OP in a wide range of respective parameters. The package has been used to analyze experimental data on differential cross sections.</p>	

3. Nonstationary generalized TASEP in KPZ and jamming regimes

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The totally asymmetric simple exclusion process (TASEP) is a well-known exactly solvable model, which belongs to the Kardar-Parisi-Zhang (KPZ) universality class [1]. Despite very simple formulation, it has a non-trivial behavior. We investigate discrete time TASEP with generalized update (GTASEP) [2]. In addition to the usual discrete time dynamics and exclusion interaction the GTASEP has an extra parameter responsible for an attractive-like interaction that enhances clustering of particles. As the parameter varies in its range, the model transforms from the discrete time TASEP with parallel update to what we call the deterministic aggregation (DA) regim. The case of infinite lattice geometry was considered for two types of initial condition. We study functional forms of the distributions in the so called "scaling limit". For moderate value of attraction parameter, we obtain the well-known Airy processes [3-4]. For large values of attraction parameter, we describe the crossover between the KPZ and non-KPZ scaling behaviors in the cases when the KPZ universality breaks down [4].

1. K. Kardar, G. Parisi, Y.Z. Zhang. Dynamic scaling of growing interfaces. Phys. Rev. Lett.56:889.892 (1986)
2. A.E. Derbyshev, S.S. Poghosyan, A.M. Povolotsky and V.B. Priezzhev, The totally asymmetric exclusion process with generalized update J. Stat. Mech. (2012) P05014
3. A.E. Derbyshev, A.M. Povolotsky, V. B. Priezzhev, Emergence of jams in the generalized TASEP Phys. Rev. E. 91, 022125 (2015)
4. T. Sasamoto, Spatial correlations of the 1D KPZ surface on a flat substrate, Journal of Physics A General Physics 38(33)
5. M. Prahofer and H. Spohn. Scale invariance of the PNG droplet and the Airy process. J. Stat. Phys. 108.5-6 (2002), pp. 1071–1106.
6. A E Derbyshev, A M Povolotsky, Nonstationary generalized TASEP in KPZ and jamming regimes.

4. CORD (Closed ORbit Dynamics): A new field map evaluation tool for cyclotron particle dynamics

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The main components of the CORD (Closed ORbit Dynamics) code used in the conceptual design of the SC230 cyclotron are presented. SC230 is a compact superconducting isochronous cyclotron for proton therapy recently proposed at JINR. Obtaining the maximum amount of information from field maps without having to perform time-consuming beam tracking is useful for the magnet and accelerating system design. The CORD code enables particle dynamics analysis based on a combination of magnetic field map analysis with electric field map analysis.

5. The influence of external radiation on the Josephson junction + nanomagnet system

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We observe Kapitza pendulum effects in the dynamics of a nanomagnet coupled to a Josephson junction and under external periodic drive. In the absence of the external influences, the direction of the magnetic moment of the nanomagnet m is along the y direction: $m = (0, 1, 0)$. When the interaction is turned on, the Josephson oscillations and the oscillating external drive—which have frequencies much higher than the oscillation frequency of the nanomagnet in the absence of perturbations—play the role of the oscillations of the suspension point of the Kapitza pendulum. The high frequency oscillations change the position of stability of the nanomagnet from $(0, 1, 0)$ to $(0, 0, \pm 1)$, as the amplitude or the frequency of the external perturbation changes. We perform both, analytical calculations and numerical simulations, and obtain a very good agreement between them.

6. Distributed information and computing infrastructure of the JINR Member State organizations

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The integration of computing power of the Joint Institute for Nuclear Research (JINR) Member State organizations into a unified distributed information and computing infrastructure is an important and topical task, the solution of which would significantly reduce the time of research with obtaining significant scientific results. This paper describes the motivation of creating the distributed cloud environment, deployed on the basis of the resources of the JINR Laboratory of Information Technologies and some JINR Member State organizations, and the approach it is based on, as well as outlines plans for using and developing the created infrastructure.

7. Rethinking α -RuCl₃

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We argue that several empirical constraints strongly restrict parameters of the effective microscopic spin model describing α -RuCl₃. In particular, such constraints dictate a substantial positive off-diagonal anisotropic coupling, $\Gamma' > 0$, not anticipated previously. The renormalization by quantum fluctuations allows to reconcile larger values of the advocated bare parameters with their earlier assessments and provides a consistent description of the field evolution of spin excitations in the paramagnetic phase. We assert that large anisotropic terms inevitably result in strong anharmonic coupling of magnons, necessarily leading to broad features in their spectra due to decays, in accord with the observations in α -RuCl₃. Using duality transformations, we explain the origin of the pseudo-Goldstone mode that is ubiquitous to the studied parameter space and is present in α -RuCl₃.

8. Information system for analyzing behavioral and morphological changes in the central nervous system in the study of the effects of ionizing radiation and other factors (joint project of MLIT and LRB JINR)

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The information system (IS) under development will allow one to combine and structure data of different types from different experiments and experimental groups into a unified information space that can provide both the convenience of storing and accessing data and a set of advanced (relevant) algorithmic procedures for data analysis automation to solve problems related to the diagnosis of different diseases of the central nervous system, which remain generally open and insufficiently studied, including at the current stage of the development of medicine.

The IS being developed on the basis of machine and deep learning methods and neural network approaches will ensure storage and access to experimental data in a form convenient for complex statistical analysis. The use of neural networks and machine learning algorithms in the framework of the given IS will allow one to solve complex problems of medical diagnosis and non-standard tasks of pathomorphologists in the study of histological preparations, reducing time and energy costs and largely eliminating the human factor.

The end-effect of the introduction of this system will be the systematisation of the accumulated experimental results, the identification of hidden patterns manifested in the response of biological systems to the effects of damaging factors. The use of IS will lead to a significant simplification and acceleration of the diagnosis of CNS pathologies, and in the particularly, the development of effective methods of prevention and protection against ionizing radiation.

9. Service for parallel computing on MICC resources

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The JINR Multifunctional Information and Computing Complex (MICC) provides a number of computing resources operated by diverse systems with different user interfaces. Mastering all the interfaces can be challenging for users due to the differences in the architecture and user interfaces of these systems. A cloud service was developed at the Laboratory of Information Technologies with the goal to abstract from the complexities of the MICC components by providing a problem-oriented web interface with unified access to the MICC computing resources. Its current state and future developments are presented.

10. Manifestation of Resonance Features and Shapiro steps on the IV- characteristic of annular system of Josephson Junctions

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We have investigated the phase dynamics of an annular system of parallel Josephson junctions (JJs) under the influence of external electromagnetic radiation [1,2]. Current-voltage characteristics (CVC) and time dependences of the magnetic field are calculated for different values of the base current. It is shown that in the presence of a trapped fluxon, Shapiro steps appear as a result of frequency locking between external radiation and the periodic motion of the trapped fluxon. It was also demonstrated that above the branch corresponding to the trapped fluxon, Shapiro steps do not appear on the I-V characteristic.

References:

1. I. R. Rahmonov, J. Tekic, P. Mali, A. Irie and Yu. M. Shukrinov, AC-driven annular Josephson junctions: The missing Shapiro steps, *Phys. Rev. B*, 101, 024512 (2020).
2. I. R. Rahmonov, J. Tekic, P. Mali, A. Irie, A. Plecenik, Yu. M. Shukrinov, Resonance phenomena in an annular array of underdamped Josephson junctions, *Phys. Rev. B*, 101, 174515 (2020).

11. Studies of the Wigner quasiprobability distributions

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The Wigner quasiprobability distribution, or simply the Wigner function (WF), provides qualitative information on many quantum phenomena occurring in diverse physical systems. In contrast to the classical statistical probability distribution, the WF takes negative values for some quantum states, and this is interpreted as an evidence of non-classicality, or quantumness. Here, based on the recently elaborated method of construction of the WF of a finite-dimensional system, the following measures/indicators for quantification of non-classicality of a finite-dimensional system are discussed:

1. KZ indicator δ_N introduced by A. Kenfack and K. Zyczowski and based on the volume of the negative part of the WF;
2. global indicator Q_N defined as a relative volume of the subspace $\mathcal{O}[\mathfrak{P}_N^{(+)}] \subset \mathcal{O}[\mathfrak{P}_N]$ of the unitary orbit space \mathcal{O}_N of a quantum system where the WF is positive.

Both measures are exemplified by considering the Hilbert-Schmidt ensemble of qubits and qutrits, while for the global indicator the Bures and Bogoliubov-Kubo-Mori metrics are also considered.

12. JINR Open Access Institutional Repository on the JOIN² Software Platform

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JOIN² (<https://join2.de>) is a shared repository infrastructure that brings together eight research institutes for the development of a full-fledged scholarly publication database and repository based on the Invenio v1.1 open source framework for large-scale digital repositories.

The JINR document server (JDS – publications.jinr.ru) is an information system representing an Open Access institutional repository of articles, preprints and other materials that reflect and facilitate research activities at JINR. The goals of JDS are to store JINR scientific information resources and provide effective access to them.

In 2019, a Memorandum of Understanding between JINR and DESY, where JOIN² is one of the cooperative projects, was signed (*Appendix 1* to the Cooperation Agreement between DESY and the Joint Institute for Nuclear Research). The pre-production version based on the JOIN² project software is available at it-jds-join2.jinr.ru.

When joining the JOIN² project, enhancements required to handle the Cyrillic alphabet for the correct display of authority records were implemented. This enhancement is also applied to other national languages. Web forms to input publications were improved taking into account types of JINR publications. The authority records of the Topical plan for JINR research and international cooperation are being downloaded to link publications with funding sources. Support of login via unified database of JINR users was implemented in JDS.