XXIX DAVYDOV READINGS

in theoretical physics
dedicated to 50 years of the Davydov's soliton

December 21, 2023, Kyiv, Ukraine
Bogolyubov Institute for Theoretical Physics
of the National Academy of Sciences of Ukraine [1]

http://bitp.kiev.ua/news

ABSTRACTS

1* *Participation of the invited guests Erik Aurell, Massimo Vergassola and Irene Giardina is part of the initiatives dedicated by the European Physical Society to strengthening scientific ties with the Ukrainian physics community.*

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Statistical genetics in and out of quasi-linkage equilibrium

Erik Aurell

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The phase of quasi-linkage equilibrium (QLE) in population biology was discovered by Kimura in 1965. This phase, which has many similarities to a thermal equilibrium state in statistical mechanics, describes a population evolving due to the mutations, recombination, natural selection and, possibly, genetic drift. A QLE phase exists at sufficiently high recombination rate and/or mutation rates with respect to selection strength. I will discuss how in QLE it is possible to infer the epistatic parameters of the fitness function from the knowledge of the (dynamical) distribution of genotypes in a population. I will further discuss the breakdown of the QLE regime for high enough selection strength, and a new phase where variability persists in the population without either fixating or disappearing. I will show data on SARS-CoV-2 sequences acquired during the pandemic and deposited in the GISAID repository, and discuss the use of such data.

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Cytoplasmic fluid dynamics

Massimo Vergassola

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50 years of the Davydov's soliton

Larissa Brizhik

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I will give a short review of theory of the Davydov's solitons. Special attention will be given to the role of Davydov's solitons in charge and energy transport processes on macroscopic distances in biological and physical systems, including novel materials used in bioimicring nanotechnologies. Some aspects of the nonlinear mechanisms of the experimentally proved non-thermal impact of external electromagnetic fields on biological systems will e discussed.

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The polarization mechanism of bacterial movement in the aquatic environment

Oleksandr Chernyak and Bohdan Lev

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The main goal of the presentation is to propose and illustrate a new possible model of bacterial movement in the aquatic environment. For this goal, the hydrodynamics of the active substance will be considered, taking into account the change in the polarization of both the environment and the bacterium itself. A possible explanation of the light-induced movement of bacteria in the aquatic environment is proposed. The explanation is based on the effects of the polarization motion of the surface of an individual bacterium. The polarization motion is due to the formation of a heterogeneous distribution of dipole moments, which are created by light and individual globules with different refractive indices. Due to these effects, an uneven distribution of polarization is created, which can move along or rotate and lead to repulsion of the liquid where the bacteria themselves are located. This is a type of turbine effect without attachment or polarization current with a change in the local polarization of the medium. We offer promising extensions for a more realistic explanation of the mechanisms of bacterial movement in the aquatic environment.

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DNA-polyamine interactions: Conformational insights

Sergiy Perepelytsya

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DNA is the strong polyelectrolyte due to the negatively charged phosphate groups in its double helical structure. In the aqueous solutions, the charges of DNA phosphates are neutralized by the positively charged ions (counterions). Natural polyamines (putrescine^{2+}, spermidine^{3+}, spermine^{4+}) are recognized as the most abundant organic counterions of DNA in the cell nucleus. Among others, the conformational flexibility of polyamines is an essential property for the formation of complexes with DNA. Yet, the characterization of the conformational space of polyamines has not been fully elucidated. In the present work, we have shown how the interactions between spermidine^{+} and the DNA double helix induce significant conformational variations in the polyamine molecule [1]. Specifically, we found that DNA induces conformations that are not observed in solution. A detailed study of the most compact conformation of the polyamine in connection with the interaction with the DNA duplex is presented [2]. The analysis reveals that anomalous bent conformations of the spermidine^{+} molecule result from the interaction of all three amino groups of the polyamine with the DNA phosphate groups on the minor groove side of the double helix. The changes in dihedral angles of the bent spermidine^{+} molecule can be explained in terms of conformational transformations of six- and seven-membered rings, analogous to cyclohexane and cycloheptane. The analysis of the position of spermidine^{+} molecule along the DNA surface reveals a sequence specificity of this binding mode, with a marked preference for the narrow minor groove of A-tracts. The formation of the anomalous bent conformations of spermidine^{+} in the complex with the DNA double helix can be of paramount importance in understanding the mechanisms underlying DNA biological function.

1. Perepelytsya S., Vasiliu T., Laaksonen A., Engelbrecht L., Brancato G., Mocci F. J. Molec. Liq., 389, 122828 (2023). https://doi.org/10.1016/j.molliq.2023.122828
2. Perepelytsya S., Vasiliu T., Laaksonen A., Engelbrecht L., Mocci F. Low Temperature Physics, submitted.

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Band structure transformation of the avoided crossing type in impure graphene

Yuriy Skrypnyk
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It is demonstrated that weakly bound impurity centers, described by the Fano model, can yield sharp resonance states near the Dirac point in the electron spectrum of graphene. Consequently, the electronic band structure of graphene undergoes a transformation of the avoided crossing type on increasing the concentration of these impurities. The stated transformation evolves in the neighborhood of the impurity resonance energy and unfolds in a threshold manner, i.e., it occurs when the impurity concentration exceeds a specific critical value, which is determined by the mutual spatial overlap of individual impurity states. In contrast to the already known cases of such band structure transformations, it manifests a new impurity Dirac point in the spectrum. In addition, it features a concentration broadening domain, or a mobility gap, of a reduced width around the impurity resonance energy. Thus, by controlling the Fermi level position in the disordered system, it should be possible to observe a metal-insulator transition when the Fermi level enters the mobility gap and, afterward, a re-entrant insulator-metal transition when it exits out of the gap.

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Out of equilibrium response, dissipation and control in flocking systems

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Flocking systems are known to be strongly out of equilibrium. Energy input occurs at the individual level to ensure self-propulsion, and the individual motility in turn contributes to ordering, enhancing information propagation and strengthening collective motion. However, even beyond ordering, a crucial feature of natural aggregations is response. How, then, off-equilibrium features affect the response of the system?

In this talk, I will address this issue both from an empirical and a theoretical perspective. I will first summarize what we know from experiments on natural swarms and flocks, and show that out of equilibrium effects are stronger in one case than in the other. Then I will consider a minimal model of flocking and investigate theoretically and numerically response behavior. Violations of equilibrium fluctuation-dissipation relations occur both at the local and at the global level and their amount peaks at the ordering transition, exactly as for the entropy production rate. Entropy is always produced locally. However, cooperative mechanisms close to the transition spread off-equilibrium effects to the whole system, producing an out of equilibrium response on the global scale. This picture reconciles nicely with what is observed in the data, providing an explanatory framework for natural systems.