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Book of Abstracts

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Session 2 / **101**

Thermodynamic activation energy for self diffusion and order-order relaxation in intermetallic compounds: atomistic model and Monte Carlo simulations

Author: Rafal Abdank-Kozubski[1]

Co-authors: Andrzej Biborski [2]; Graeme E. Murch [3]; Irina V. Belova [3]; Piotr Sowa [1]

[1] *M. Smoluchowski Institute of Physics, Jagiellonian University in Krakow*

[2] *AGH University of Science and Technology Academic Centre for Materials and Nanotechnology*

[3] *Centre for Mass and Thermal Transport in Engineering Materials, School of Engineering, The University of Newcastle, Callaghan, Australia*

Corresponding Author: rafal.kozubski@uj.edu.pl

Self-diffusion and the 'order order' relaxation process in intermetallic compounds is described in terms of effective atomic jump frequencies and the current degree of chemical long-range order. It is demonstrated that the thermodynamic activation energies of self-diffusion and the 'order-order' relaxation can be expressed in terms of the activation energies of more elementary processes. As the derived expressions differ from each other, the values of the thermodynamic activation energies for self-diffusion and the 'order order' relaxation can be different although both processes are controlled by the same vacancy-mediated elementary atomic jumps.
In order to assess the the validity of the derived formulae different B2-ordering binary systems are simulated. The results of the computer experiments are in good agreement with the tested formulae. It is shown that the relationship between the activation energies observed in triple defect B2-ordering binaries, where the value of the activation energy for order-order relaxations is substantially lower than that for self-diffusion, does not hold in the case of non-triple-defect binaries. Using the tested formulae, the origin of the effect is elucidated and attributed to the atomistic origin of the tendency for triple-defect disordering.

P. Sowa, A. Biborski, M. Kozłowski, R. Kozubski, I.V. Belova, G.E. Murch: Atomistic origin of the thermodynamic activation energy for self diffusion and order-order relaxation in intermetallic compounds. Part I and Part II, Philos.Mag., **97**, 1361-1374, 1375-1397 (2017).

Session 5 / **51**

Quantum model of self-oscillations in chemical engines

Author: Robert Alicki[1]

[1] *University of Gdansk*

Corresponding Author: fizra@univ.gda.pl

A standard textbook picture of solar, thermoelectric and fuel cells based on a direct transformation of light, heat or chemical energy into a direct current (DC) contradicts the basic principles of electrodynamics and thermodynamics. The proposed solution of this problem involves a single oscillating degree of freedom called work reservoir (depository) or a piston, which executes self-oscillations fed by a constant energy supply. In the mentioned examples, it is a mode of plasma oscillations and the resulting charge oscillations are finally rectified to DC by a diode mechanism. The onset of self-oscillations is illustrated by a simple quantum Markovian model of a harmonic oscillator coupled to chemical reservoirs. The proper definition of work output is discussed in terms of ergotropy.

Session 2 / **46**

Quantum first detection time

Author: Eli Barkai[1]

Co-authors: David Kessler [1]; Felix Thiel [1]

[1] *Bar-Ilan University, Israel*

Corresponding Author: barkaie@biu.ac.il

We investigate the quantum first detection problem for a quantum walk
using projective measurement postulates.
A simple relation between the measurement free state function |psi> and |phi>_n is obtained,
the latter
is the first detection amplitude at the n-th attempt. This relation is the quantum renewal equation, its classical counter part is widely used to find statistics of first passage time for random walks and Brownian motion. We investigate statistics of first detection for open and closed systems (first arrival or passage is not well defined in quantum theory). For closed systems, like a ring, with a
translation invariant Hamiltonian, we find Zeno physics, optimum sampling times, critical sampling effect related to revivals, dark states, and quantisation of the mean detection time. For a quantum walk on the line, with particle starting on |x_i> and detected on the origing |0>, with a tight-binding Hamiltonian with hops to nearest neighbours, we find the detection probability decays like (time)^(-3) with super imposed quantum oscillation, thus the quantum exponent is double its classical counter part. The Polya problem is discussed, and it is found that in one dimension the total detection probability, does not depend on the initial distance of the particle from detector, though survival of the particle is not unity. There is an optimal sampling time which maximises the
total detection probability.

Joint work with Harel Fridman, David Kessler, and Felix Thiel.

Session 8 / **61**

Looping and direct transit in Brownian particle escape from force-biased and entropic traps

Author: Sergey Bezrukov[1]

Co-authors: Alexander Berezhkovskii [1]; Leonardo Dagdug [2]

[1] *National Institutes of Health, Bethesda, MD 20892, USA*

[2] *National Institutes of Health, Bethesda, MD 20892, USA and Universidad Autonoma Metropolitana-Iztapalapa, 09340 Mexico City, Mexico*

Corresponding Author: bezrukos@mail.nih.gov

Recent experiments with single biological nanopores, as well as single-molecule fluorescence spectroscopy and pulling studies of protein and nucleic acid folding raised a number of questions that stimulated theoretical and computational studies of the barrier crossing dynamics. We focus on trajectories of Brownian particles that escape from traps either in the presence of an external force or an entropy potential of a cone. To gain new insights into the escape dynamics, we divide the trajectories into two segments: a looping segment, when a particle unsuccessfully tries to escape returning to the trap bottom, and a direct-transit segment, when it finally escapes moving without returning to the bottom. Analytical expressions are derived for the Laplace transforms of the probability densities of the durations of the two segments. These expressions are used to find the mean looping and direct-transit times as functions of the external force or entropy potential. It turns out that the force/potential dependences of the two mean times are qualitatively different. The mean

looping time monotonically increases with the force pushing the particle to the trap bottom or with the increasing entropic barrier at the exit. In contrast to this intuitively appealing result, the mean direct-transit time shows rather counterintuitive behavior: it is reduced by force application independently of whether the force pushes the particles to the trap bottom or to the trap exit and it turns out to be insensitive to the entropy potential.

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Quantum Brownian Motion

Author: Paweł Bialas[1]

Co-author: Jerzy Łuczka [1]

[1] *Department of Theoretical Physics, University of Silesia*

Corresponding Author: pawel.bialas@smcebi.edu.pl

Models which contain quantum particle coupled to its environment were analysed many times over recent years or even decades. Nonetheless this old and seemingly well known problem contains some unknown aspects and have not been solved in the general case. Furthermore by analysing behaviour of quantum Brownian motion one could attempt to find answer for many fundamental questions concerning the very essence of the quantum world, investigate transport phenomena or consider the nature and properties of quantum information.
The topic of quantum Brownian motion is fundamental for many fields of physics, for instance in statistical physics, condensed matter and atomic physics.
There are plenty of methods for analysing such systems for instance path integrals method, van Kampen method or generalised Langevin equation method. In our considerations we utilise the last listed method and as a starting point in our analysis we took quantum fluctuation-dissipation theorem.
We would like to present some of interesting properties exhibited by such systems and exact, analytical results which we have obtained. In our investigations we were focused mainly on the kinetic energy of Brownian particle in long-time limit and general formula for autocorrelation function.

Session 12 / **106**

A Boltzmann-distribution-equivalent for Levy noise and how it leads to thermodynamically consistent epicatalysis

Author: Martin Bier[1]

[1] *East Carolina University*

Corresponding Author: bierm@ecu.edu

Nonequilibrium systems commonly exhibit Levy noise. This means that the distribution for the size of the Brownian fluctuations has a “fat” power tail. Large Brownian kicks are then more common as compared to the ordinary Gaussian distribution that is associated with equilibria.

We consider a two-state system, i.e. two wells and in between a barrier that is sufficiently high for a barrier crossing to be a rare event. When the noise is Levy, we do *not* get a Boltzmann distribution

between the two wells. Instead we get a situation where the distribution between the two wells also depends on the height of the barrier that is in between.

A catalyst, by lowering the barrier between two states, can speed up the establishment of an equilibrium. It will, however, not change the equilibrium distribution. In an environment with Levy noise, on the other hand, we have the possibility of epicatalysis, i.e. a catalyst effectively altering the steady state distribution between two states by changing the barrier height. We discuss how this idea may possibly apply to nuclear reactions and to biochemical reality in a living cell.

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ARC4 stream cipher as a nonlinear mixing dynamical system

Author: Teodor Buchner[1]

[1] *Faculty of Physics, Warsaw University of Technology*

Corresponding Author: buchner@if.pw.edu.pl

Due to outspread of WiFi technology, which utilized stream ciphers, ARC4 has once become the most widespread stream cipher in the world. The idea of the cypher is to use a deterministic dynamics, with strong mixing properties in order to produce a pseudorandom trajectory of symbols, identically distributed, with minimal correlations. A pair of ARC4 sharing common initial condition (secret key) is used to produce the same trajectory on the encrypting and decrypting side.

The aim of this contribution is to show a few results, which may be obtained if we apply standard techniques of nonlinear dynamics to a trajectory generated by some cryptographic system.

The first effect we show is a relation between Renyi entropy distribution of the pseudorandom string and the quality of the key. Various strategies for key selection introduce variability in the minimum and the peak of entropy distribution.

The second effect we show is the nonuniform distribution of sum of two consecutive samples (a digraph). Families of digraphs revealing certain anomalies were known before, but application of the return map, shows a nonuniform probability certain area of phase space in Takens reconstruction. Hence, the generator is distinguishable from random, although the timeseries look completely random.

Some successful attacks upon RC4 have relied on a fact, quite nonlinear in spirit, that within the transient phase, the system did not loose information about its initial conditions fast enough, which produced correlations, which were utilized to reveal the key, and decipher the message. A lack of standard nonlinear operation: i.e. omission of transients led to compromitation of the whole WiFi technology (WEP). Current findings confirm that application of nonlinear techniques in cryptology may provide interesting results.

Session 12 / **58**

Microscopic derivation of coloured Lévy flights in active swimmers' suspensions

Authors: Adrian Baule[1]; Andrea Cairoli[2]; Kiyoshi Kanazawa[3]; Tomohiko G. Sano[4]

[1] *Queen Mary University of London*

[2] *Imperial College London*

[3] *Institute of Innovative Research, Tokyo Institute of Technology*

[4] *Department of Physical Sciences, Ritsumeikan University*

Corresponding Author: andrea.cairoli11@imperial.ac.uk

The motion of a tracer particle in a complex medium typically exhibits anomalous diffusive patterns, characterised, e.g, by a non-liner mean-squared displacement and/or non-Gaussian statistics.
Modelling such fluctuating dynamics is in general a challenging task, that provides, despite all, a fundamental tool to probe the rheological properties of the environment.
A prominent example is the dynamics of a tracer in a suspension of swimming microorganisms, like bacteria, which is driven by the hydrodynamic fields generated by the active swimmers.
For dilute systems, several experiments confirmed the existence of non-Gaussian fat tails in the displacement distribution of the probe particle, that has been recently shown to fit well a truncated Lévy distribution.
This result was obtained by applying an argument first proposed by Holtsmark in the context of gravitation: the force acting on the tracer is the superposition of the hydrodynamic fields of spatially random distributed swimmers.
This theory, however, does not clarify the stochastic dynamics of the tracer, nor it predicts the non monotonic behaviour of the non-Gaussian parameter of the displacement distribution.
Here we derive the Langevin description of the stochastic motion of the tracer from microscopic dynamics using tools from kinetic theory.
The random driving force in the equation of motion is a coloured Lévy Poisson process, that induces power-law distributed position displacements.
This theory predicts a novel transition of their characteristic exponents at different timescales. For short ones, the Holtzmark-type scaling exponent is recovered; for intermediate ones, it is larger.
Consistently with previous works, for even longer ones the truncation appears and the distribution converge to a Gaussian.
Our approach allows to employ well established functional methods to characterize the displacement statistics and correlations of the tracer. In particular, it qualitatively reproduces the non monotonic behaviour of the non-Gaussian parameter measured in recent experiments.

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Epidemics spread in heterogeneous populations

Author: Karol Capała[1]

Co-author: Bartłomiej Dybiec [1]

[1] *Institute of Physics, Jagiellonian University*

Corresponding Author: karol.capala@student.uj.edu.pl

Individuals building populations are subject to variability. This variability affects progress of epidemic outbreaks, because individuals tend to be more or less resistant. Agents also differ with respect to their recovery rate. Here, properties of the SIR model in inhomogeneous populations are studied. It is shown that a small change in model's parameters, e.g recovery or infection rate, can substantially change properties of final states which is especially well-visible in distributions of the epidemic size.
In addition to the epidemic size and radii distributions first passage time properties of epidemic outbreaks are explored.

K. Capala, B. Dybiec, Eur. Phys. J. B 90 85 (2017).

Session 3 / **95**

Harmonic spectral components in time sequences of Markov correlated events with an application to EEG and MEG signals

Authors: Anna Carbone[1]; Piero Mazzetti[1]

[1] *Politecnico di Torino*

Corresponding Author: anna.carbone@polito.it

The talk is addressed to the analysis of time sequences of Markov correlated events give rise to a line power spectrum having a relevant physical interest. In particular, Markov matrices able to represent closed loop sequences of events with arbitrary distribution, generated in a steady physical condition, generate a large set of line spectra, covering a very broad frequency range. The spectral lines is given by a matrix equation based on a generalized Markov matrix involving the Fourier transform of the distribution functions representing the time intervals between successive events of the sequence. The theoretical power spectra is then applied to describe the emergence of a broad set of waves found in the electro and magneto-encephalograms, whose frequency ranges from 0.5 to about 40 Hz, in terms of the effects produced by chains of firing neurons within the complex neural network of the brain. Synchronized closed loop sequences of firing neurons are considered and a few numerical simulations are reported.

Session 8 / **89**

Novel ordered phases in coupled driven systems: large compact clusters and fast dynamics

Author: Sakuntala Chatterjee[1]

Co-authors: Mustansir Barma [2]; Shauri Chakraborty [1]; Sukla Pal [1]

[1] *S.N. Bose National Centre for Basic Sciences, Kolkata, India*

[2] *TIFR Hyderabad*

Corresponding Author: sakuntala.chatterjee@gmail.com

We demonstrate particle clustering on macroscopic scales in a coupled nonequilibrium system where two species of particles are advected by a fluctuating landscape and modify the landscape in the process. The phase diagram generated by varying the particle-landscape coupling, valid for all particle density and in both one and two dimensions, shows novel nonequilibrium phases. While particle species are completely phase separated, the landscape develops macroscopically ordered regions coexisting with a disordered region, resulting in coarsening and steady state dynamics on time scales which grow algebraically with size, not seen earlier in systems with pure domains.

(1) Large compact clusters and fast dynamics in coupled nonequilibrium systems,
S Chakraborty, S Pal, S Chatterjee, M Barma, Phys Rev E **93**, 050102(R) (2016).

(2) Ordered phases in coupled nonequilibrium systems: static properties, S Chakraborty, S Chatterjee, M Barma, Phys Rev E (accepted), arXiv 1704.03309.

(3) Ordered phases in coupled nonequilibrium systems: dynamic properties, S Chakraborty, S Chatterjee, M Barma, Phys Rev E (accepted), arXiv 1704.03320.

Non - equilibrium translocation dynamics of end pulled polymer chains

Author: Srabanti Chaudhury[1]

Co-author: Bappa Ghosh [1]

[1] *Indian Institute of Science Education and Research*

Corresponding Author: srabanti@iiserpune.ac.in

The translocation dynamics of a polymer chain driven through a nanopore by an external bias between the cis and trans side of the chain is a far from equilibrium process. With the emergence of single molecule techniques, the translocation of a polymer can be studied by applying a mechanical force on one end of the polymer by using an optical or a magnetic tweezer. In this work, we consider the translocation dynamics of a polymer chain pulled through a nanopore with a strong driving force applied at the head end of the chain using Langevin dynamics simulations [1]. The translocation time distribution, the mean translocation time and waiting time distributions are calculated. The waiting time as a function of the monomer number is non- monotonic in nature which clearly indicates that the translocation is a far from equilibrium process. The velocity profile of the monomer at different times shows that translocation process is accompanied by the propagation of tension front along the polymer chain [2]. The distribution of waiting times reaches a maximum when the tension front has propagated to the last monomer bead. Our simulation results are supported by theoretical studies by using the iso- flux tension propagation theory (IFTP) of driven translocation to derive explicit equations of motion for the dynamics [3,4], and include the friction term arising from the trans side of the subchain. The theoretical results are in excellent agreement with the molecular dynamics simulations. We obtain exact analytical expression for the scaling behavior of the average translocation time as a function of the chain length and the exteranal driving force.

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Session 7 / **18**

Understanding cooperativity and dynamic disorder in fluctuating enzymes at the single molecule level

Author: Srabanti Chaudhury[1]

Co-author: Divya Singh [1]

[1] *Indian Institute of Science Education and Research*

Corresponding Author: srabanti@iiserpune.ac.in

Single molecule techniques allow researchers to study not only the average reaction rates but also the statistics of single molecule transitions in the context of enzymatic reactions. Such measurements show that the slow fluctuation between enzyme conformers can lead to fluctuations in the rate constants of the reaction, a phenomenon known as dynamic disorder [1]. The most accessible characteristics of reactivity fluctuations in individual enzyme molecules relate to the second moment of turnover time statistics and is defined by the randomness parameter. Measurement of this quantity can serve as an indicator for dynamic disorder in the catalytic step of the reaction. Such enzymatic fluctuations can also lead to deviation in Michaelis- Menten behavior of the reaction rates

and the emergence of dynamic cooperativity in single enzymes. In this talk I will discuss about a few such biologically relevant enzyme reaction schemes with multiple binding sites and slow fluctuations between the binding sites. I will propose a simple analytical model based on the first passage time distribution between successive catalytic turnover events that can be used to calculate the average reaction rate and obtain closed-form analytical expressions of the randomness parameter in terms of constant parameters [2, 3]. Our results confirm that slow fluctuations between the free enzyme conformers can lead to dynamic cooperativity whereas dynamic disorder at high substrate concentration is determined only by the slow fluctuations between the enzyme – substrate conformers [4]. Our theoretical findings are well supported by comparison with experimental data on the single enzyme beta-galactosidase [5].

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Session 5 / **56**

Brownian yet non-Gaussian Diffusion

Author: Aleksei Chechkin[1]

Co-authors: Flavio Seno [2]; Igor Sokolov [3]; Ralf Metzler [4]

[1] *Akhiezer Institute for Theoretical Physics*

[2] *University of Padova*

[3] *Humboldt University Berlin*

[4] *University of Potsdam*

Corresponding Author: aleksei.chechkin@gmail.com

A growing number of biological, soft, and active matter systems are observed to exhibit normal diffusive dynamics with a linear growth of the mean-squared displacement, yet with a non-Gaussian distribution of increments. Based on the Chubinsky-Slater idea of a diffusing diffusivity, we here establish and analyze a minimal model framework of diffusion processes with fluctuating diffusivity. In particular, we demonstrate
the equivalence of the diffusing diffusivity process with a superstatistical approach with a distribution of diffusivities, at times shorter than the diffusivity correlation time. At longer times, a crossover to a Gaussian distribution with an effective diffusivity emerges. Specifically, we establish a subordination picture of Brownian but non-Gaussian diffusion processes, which can be used for a wide class of diffusivity fluctuation statistics. Our results are shown to be in excellent agreement with simulations and numerical evaluations.

Aleksei V. Chechkin, Flavio Seno, Ralf Metzler, and Igor M. Sokolov, PHYSICAL REVIEW X 7, 021002 (2017).

Session 1 / **153**

Life at the edge, complexity and criticality in biological function

Author: Dante Chialvo[1]

[1] *Center for Complex Systems & Brain Sciences (CEMSC3). Universidad Nacional de San Martin & CONICET. San Martin, Buenos Aires, Argentina*

Corresponding Author: dchialvo@conicet.gov.ar

The organization of biological form and function is a classic problem, cut-crossing disciplines, which include a variety of complex spatiotemporal patterns. Historically, work focussed first into the understanding of self-organization and later attention shifted to scale-free collective fluctuations, many of them shown to correspond to critical phenomena. In that context, I will review our work on critical dynamics across several scales uncovering novel understanding of proteins, mitocondria and brain function.

Session 0 / **186**

Marian Smoluchowski his life and works

Author: Bogdan Cichocki[1]

[1] *Instytut Fizyki Teoretycznej Uniwersytetu Warszawskiego*

Corresponding Author: cichocki@fuw.edu.pl

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Studies on the structure - diffusion relationship for polymer membranes with different surface morphology

Authors: Anna Strzelewicz[1]; Gabriela Dudek[1]; Michał Cieśla[2]; Monika Krasowska[1]

[1] *Department of Physical Chemistry and Technology of Polymers, Silesian University of Technology, Gliwice, Poland*

[2] *M. Smoluchowski Institute of Physics, Jagiellonian University, Kraków, Poland*

Corresponding Author: michal.ciesla@uj.edu.pl

The relationship between membranes morphology, which is characterized by different parameters, and the characteristics of diffusive transport in the membranes is studied. Membranes comprising of polymer with dispersed inorganic fillers are characterized by polymer matrix density, its fractal dimension, the average size of domains and average number of near obstacles. Diffusive transport is investigated by simulation of a particle motion in the membrane environment. Comparison of diffusion driven by Gaussian random walk and Lévy flights shows that the effective diffusion exponent at long time limit is subdiffusive and it does not depend on the details of the underlying random process causing diffusion. Additionally, the determined ergodicity breaking parameter shows non-ergodic behavior in the case of structures that consist of a mix of a large number of small obstacles. Analysis of several parameters describing membrane structure shows that the most important factor for diffusion character is the average size of domain penetrated by diffusing particle. Obtained results might be useful in the design and preparation of the membrane structures with specific diffusion properties.

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Designing of the membrane's morphology with prescribed structure and diffusion properties

Authors: Anna Strzelewicz[1]; Gabriela Dudek[1]; Michał Cieśla[2]; Monika Krasowska[1]

[1] *Department of Physical Chemistry and Technology of Polymers, Silesian University of Technology, Gliwice, Poland*

[2] *M. Smoluchowski Institute of Physics, Jagiellonian University, Kraków, Poland*

Corresponding Author: michal.ciesla@uj.edu.pl

Preparation of a membrane with prescribed properties, which can provide a chance to control mass transport and decide about the time and number of particles released from the membrane is nowadays one of great importance scientific problems. In our previous papers it was shown that at intermediate and long time-scale the diffusion type depends on the membrane structure but not on the specific process that causes the movement. The effective diffusion exponent seems to depend on an average size of domains that are penetrated by randomly moving tracers and density of obstacles [1-3]. This work describes an attempt to create an accurate computer model of a particular morphology of membrane i.e. polymeric matrix with dispersed nanoparticles. In particular to develop a computer program to design the structure of membrane with prescribed the size and shape distribution of obstacles (nanoparticles, aggregates of nanoparticles). Good qualitative and quantitative agreement can be seen between graphical output of the models and microscopy images. The presented results may be used in the design and preparation of polymeric membrane with nanofillers for separation and pervaporation process.

[1] M. Krasowska, A. Strzelewicz , A. Rybak, G. Dudek, M. Cieśla, *Structure and transport properties of ethylcellulose membranes with different types and granulation of magnetic powder*, Physica A: Statistical Mechanics and its Applications, **452** 241 (2016)

[2]M. Cieśla, E. Gudowska-Nowak, F. Sagues, I.M. Sokolov, *Tracer diffusion inside fibrinogen layers*, Journal of Chemical Phycics, **144** 044706 (2014)

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Thermodynamic approach to non-relativistic quantum mechanics

Author: Davide Cocco[1]

Co-author: Massimiliano Giona [1]

[1] *Università di Roma La Sapienza*

Corresponding Author: cocco.1487501@studenti.uniroma1.it

In this contribution we explore the derivation of quantum mechanics from a classical field theory, or more precisely from a thermodynamic approach involving two field phases. This attempt is in line with the analysis of Laughlin and Pines on the emergent characters of physical laws, including quantum physics (PNAS, 97, 2000, 28).

The first part of the presentation analyzes in detail the stochastic interpretation of quantum physics grounded on the "Advective Quantum Gauge" (AQG for short), i.e., on the equivalence between the Schrodinger and the advection diffusion equations in a Wick-rotated time.

Albeit this connection have been addressed by a huge and extensive literature, several implications of the above equivalence are fairly novel and of physical interest. Specifically:

(i) The AQG approach provides for quantum system a kinematic equation of motion (complex Langevin equation) of the form $d\mathbf{x}(t) = i\,\mathbf{v}_q(\mathbf{x}(t))\,dt + \sqrt{i\,2\,D_h}\,d\mathbf{w}(t)$ where $d\mathbf{w}(t)$ the increments of a n-dimensional real-valued Wiener process. In the absence of stochastic fluctuations, from the above model one recovers the semiclassical limit of the Newton equations of motion.

(ii) The AQG furnishes an interesting interpretation of Bohmian quantum dynamics, as a mean field theory in which quantum fluctuations are accounted for by the quantum potential which depends on the modulus of the wavefunction.

(iii) The AQG provides a way to obtain the wavefunction or the quantum propagators in a simple and efficient way from random walk simulations. This is particularly relevant for quantum problems involving many degrees of freedom.

The stochastic interpretation of quantum mechanics, and specifically the AQG approach, is essentially a particle-based description of a physical system intrinsically subjected to fluctuations. This approach shows some limitations in the presence of time-dependent (and, a fortiori} stochastic) potentials.

The second part of the presentation provides a classical field-theoretical interpretation of the Schrodinger equation, in which quantum (field) fluctuations

still play a leading role, but a quantum system is viewed as a statistical mechanical system in which two field-phases coexist.

In the present thermodynamic model we assume that a quantum system corresponds to a two-phase thermodynamic system in which a “distributed” (radiating) field coexists with a “condensed field phase”. Quantum equation of motion emerges from the interaction between the two phases by assuming a quasi steady-state approximation. As regards the condensed phase, it is at present described in a particle-like way via position and momentum.

As mentioned above, from a quasi-state approximation on the statistical description of the condensed field phase, Schrodinger equation is recovered.
More precisely, a system of hyperbolic first-order equations analogous to the statistical description of Generalized Poisson-Kac processes is derived.
The Kac limit of these equations provides the classical Schrodinger model containing the Laplacian operator accounting for the kinetic energy.

Session 2 / **158**

Dynamics of classical isolated disordered systems

Author: Leticia, F Cugliandolo[1]

[1] *Universite Pierre et Marie Curie*

Corresponding Author: leticia@lpthe.jussieu.fr

We study the dynamics of classical disordered macroscopic models completely isolated from the environment reproducing, in a classical setting, the ‘quantum quench’ protocol. We use two classes of models, distinguished by the complexity of their energy landscape. We identify quenches after which the evolution approaches a stationary state that can be associated to equilibrium at a single temperature (related to the energy change during the quench), cases in which an ageing asymptotic dynamics persists asymptotically, and quenches in which a steady state characterised by a Generalised Gibbs Ensemble is found. In the latter case we show that all the GGE effective temperatures can be obtained from the standard fluctuation dissipation relation, in the frequency domain. The parameter dependence of the asymptotic states is rationalised in terms of dynamic phase diagrams.

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[2] Laura Foini, Andrea Gambassi, Robert Konik, Leticia F. Cugliandolo Phys. Rev. E 95, 052116 (2017)

Session 2 / **109**

Variational formula for the current generating function and finite-time thermodynamic uncertainty relations

Author: Andreas Dechant[1]

Co-author: Shin-ichi Sasa [1]

[1] *Kyoto University*

Corresponding Author: andreas.dechant@outlook.com

Bounds on the current generating function for stochastic dynamics and the thermodynamic uncertainty relations that follow from them have recently attracted much attention. Here, we focus on the space-time continuous case of Langevin dynamics. We derive a variational formula for the generating function of a generalized current, which is valid at finite time, extending the previously known results for the long-time limit. We show that the proof of the recently proposed finite-time thermodynamic uncertainty relation follows from the variational formula in a straightforward way. This relation provides a universal bound on any current in a non-equilibrium steady state in terms of the entropy production. We also discuss possible extensions to the transient case and to systems with time-dependent driving.

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Phase transitions in a molecular zipper: Lee-Yang zeros and large deviation statistics

Author: Aydin Deger[1]

Co-authors: Christian Flindt [1]; Kay Brandner [1]

[1] *Department of Applied Physics, Aalto University, Finland*

Corresponding Author: aydin.deger@aalto.fi

Originally introduced to explain the behavior of a condensing gas, Lee-Yang zeros have nowadays become a universal and powerful tool for the unified description of phase transitions in equilibrium and non-equilibrium systems, see for example [1, 2]. Here, we use Lee-Yang zeros to analyze a paradigmatic model for thermal phase transitions in molecular systems. For the most simple version of this model, we explicitly calculate the Lee- Yang zeros with respect to inverse temperature. Extrapolation then allows us to infer a phase transition in the macroscopic limit, from the analysis of systems containing only a few molecular units. In a second step, we in- crease the complexity of the model. The Lee-Yang zeros can still be obtained using a recently established relation involving high-order cumulants of the energy. Finally, we show that, even when the system does not undergo a phase-transition, the Lee-Yang zeros still encode valuable physical information; they crucially determine the large deviation statistics of energy fluctuations. Specifically we show that the large deviation function generically has the form of an ellipse, whose tilt and width can be inferred from the complex Lee-Yang zeros. Our analysis reveals an interesting duality between the energy fluctuations of small-size systems in equilibrium and their phase- behavior in the thermodynamic limit [3]. To what extent this relation is valid in more complex systems, such as the two-dimensional Ising model, is a topic of future research.

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Session 3 / **11**

Characterizing rare fluctuations in soft particulate flows

Author: S. H. E. Rahbari[1]

Co-authors: Abbas Ali Saberi [2]; Hyunggyu Park [1]; Juergen Vollmer [3]

[1] *KIAS*

[2] *Tehran University*

[3] *Polito Torino*

Corresponding Author: habib.rahbari@gmail.com

Soft particulate media include a wide range of systems involving athermal dissipative particles both in non-living and biological materials. Characterization of flows of particulate media is of great practical and theoretical importance. A fascinating feature of these systems is the existence of a critical rigidity transition in the dense regime dominated by highly intermittent fluctuations that severely affects the flow properties. Here, we unveil the underlying mechanisms of rare fluctuations in soft particulate flows. We find that rare fluctuations have different origins above and below the critical jamming density and become suppressed near the jamming transition. We then conjecture a time-independent local FR, which we verify numerically, and that gives rise to an effective temperature. We discuss similarities and differences between our proposed effective temperature with the conventional kinetic temperature in the system by means of a universal scaling collapse.

Session 12 / **29**

Translational and rotational Brownian motion of particles of complex shapes

Author: Maria L. Ekiel-Jezewska[1]

Co-authors: Bogdan Cichocki [2]; Eligiusz Wajnryb [1]

[1] *Institute of Fundamental Technological Research, Polish Academy of Sciences*

[2] *Institute of Theoretical Physics, University of Warsaw*

Corresponding Author: mekiel@ippt.pan.pl

The characteristic time scales of the translational and rotational Brownian diffusion for nanoparticles are typically much smaller than time resolution of the experiments. In this case, nanoparticles can be treated as point-like, and described by the standard Brownian theory. However, for microparticles, the characteristic Brownian time scales are of the order of seconds, and therefore non-negligible in comparison to the typical time scales of the measured Brownian motion. For microparticles of complex shapes, a more general theoretical approach is needed. The exact analytical expressions for the time-dependent cross-correlations of the translational and rotational Brownian displacements of a particle with arbitrary shape have been recently derived [1,2], and it has been demonstrated how to benefit from these results while analyzing experimental data [3].

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Session 4 / 114

Isothermal Langevin dynamics in systems with power-law spatially dependent friction

Author: Oded Farago[1]

[1] *Ben Gurion University*

Corresponding Author: ofarago@bgu.ac.il

We study the dynamics of Brownian particles in a heterogeneous one-dimensional medium with a spatially-dependent diffusion coefficient of the form $D(x) \sim |x|^c$, at constant temperature. The particle's probability distribution function (PDF) is calculated both analytically, by solving Fick's diffusion equation, and from numerical simulations of the underdamped Langevin equation. At large times, the PDFs calculated by both approaches yield identical results, corresponding to subdiffusion for $c < 0$, and superdiffusion for $0 < c < 1$. For $c > 1$, the diffusion equation predicts that the particles accelerate. Here, we show that this phenomenon, previously considered in several works as an illustration for the possible dramatic effects of spatially-dependent thermal noise, is unphysical. We argue that in an isothermal medium, the motion cannot exceed the ballistic limit ($\langle x2\rangle\ t^2$). The ballistic limit is reached when the friction coefficient drops sufficiently fast at large distances from the origin, and is correctly captured by Langevin's equation.

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Population dynamics and pattern transitions in a nonlocal logistic map

Authors: André Penna[1]; Fernando Barbosa[2]; Fernando Oliveira[1]; Jefferson Cunha[3]; Keila Novais[1]; Rogelma Ferreira[4]

[1] *Universidade de Brasília*

[2] *Instituto Federal de Brasília*

[3] *Universidade Federal de Goiás*

[4] *Universidade Federal do Recôncavo da Bahia*

Corresponding Author: rogelma.maria@gmail.com

We examine the pattern solutions in a generalized nonlocal logistic map that includes spatial kernels in both growth and competition terms. We show that this map includes as a particular case the nonlocal Fisher–Kolmogorov equation, and we demonstrate the
existence of three kinds of stationary nonlinear solutions: one uniform, one cosine type that we refer to as wavelike solution, and another in the form of Gaussian. We also obtain analytical expressions that describe the nonlinear pattern behavior in the system, and we establish the stability criterion. We define thermodynamics quantities such as entropy and the order parameter. Based on this, the pattern-no-pattern and pattern–pattern transitions
are properly analyzed. We show that these pattern solutions may be related to the recently observed peak adding phenomenon in nonlinear optics.

Session 5 / **134**

A mesoscopic model for the DNA G-quadruplex stability analysis

Authors: Alessandro Fiasconaro[1]; Ana Elisa Bergues-Pupo[1]; Fernando Falo[1]

Co-authors: Irene Gutierrez [2]; José Ricardo Arias-Gonzalez [2]

[1] *Universidad de Zaragoza, Spain*

[2] *Instituto Madrileño de Estudios Avanzados en Nanociencia, Madrid, Spain*

Corresponding Author: afiascon@unizar.es

The G-quadruplexes (G4) are non-canonical secondary DNA and RNA structures composed of four guanine basis bonded each other in a quartets forming piled planes. They have been found both in vivo and in vitro cultures, and have important role in telomere end-protection, and chromosome stability. Their folding patterns and structures are also found in eukaryotic promoter regions of oncogenes, making them increasingly recognized among chemists and biologists due to their potential applications in Nanomedicine as therapeutic targets in cancer treatments.

In the last years, single-molecule techniques have attracted much attention between the scientific community and a number of groups have used it extensively to analyze the mechano-chemical behavior of DNA and RNA. Optical and magnetic tweezers, as well as Atomic Force Microscopies, are employed to characterize not only the mechanical stability and unfolding dynamics of G-quadruplexes, but also to unveil structural intermediates not accessible to ensemble-average techniques due to their relatively low occurrence.

The stability of the G-quadruplex structure is related, among the others, to the specific structural G-quadruplex conformation, and the presence of a cation between each G4 planes.
To date, many experiments have been conducted, which want to finely analyze rupture profiles in single force-extension curves.
Although the increasing number of experiments on the subject, the theoretical predictions remain difficult, due essentially to the long computational time required by atomistic simulations, which, moreover, use parameter values (for example the velocity at which one extreme of the quadruplex is pulled to induce the rupture) some orders of magnitude far away from the experimental values.

With the aim to bridge the gap between experiment and theoretical expectations, we build a mesoscopic physical model of the G-quadruplex structure with a reduced number of degrees of freedom and effective potential that permits to study the mechanical unfolding in a wider interval of time scales than those allowed in all atom simulations, in particular under different pulling velocities. The subsequent analysis on the light of the most recent stochastic theories for rupture force - as those of Bell, Dudko and Yoreo - permit the estimations of the potential barriers and positions that characterize the energy landscape of the unfolding process.

Some validation of the model with the results of experiments will be presented.

Session 4 / **154**

How to measure load-dependent kinetics of individual motor molecules without a force-clamp

Author: Henrik Flyvbjerg[1]

Co-authors: James A. Spudich [2]; Jongmin Sung [3]; Kim Mortensen [1]

[1] *Department of Micro- and Nanotechnology, Technical University of Denmark, Kongens Lyngby, Denmark*

[2] *Department of Biochemistry, Stanford University School of Medicine*

[3] *Department of Cellular and Molecular Pharmacology, The Howard Hughes Medical Institute, University of California, San Francisco*

Corresponding Author: henrik.flyvbjerg@nanotech.dtu.dk

Molecular motors are responsible for numerous cellular processes from cargo transport to heart contraction. Their interactions with other cellular components are often transient and exhibit kinetics that depend on load. Here, we measure such interactions using a new method, "Harmonic Force Spectroscopy." In this method, harmonic oscillation of the sample stage of a laser trap immediately, automatically and randomly applies sinusoidally varying loads to a single motor molecule interacting with a single track along which it moves. The experimental protocol and the data analysis are simple, fast and efficient. The protocol accumulates statistics fast enough to deliver single-molecule results from single-molecule experiments. We demonstrate the method's performance by measuring the force-dependent kinetics of individual human beta-cardiac myosin molecules interacting with an actin filament at physiological ATP concentration. We show that a molecule's ADP release rate depends exponentially on the applied load. This points to Kramer's Brownian diffusion model of chemical reactions as explanation why muscle contracts with a velocity inversely proportional to external load.

EPS / 161

Measuring effective temperatures in a Generalized Gibbs ensemble

Authors: Andrea Gambassi[1]; Jacopo De Nardis[2]; Laura Foini[2]; Leticia Cugliandolo[3]; Milosz Panfil[4]; Robert Konik[5]

[1] *SISSA Trieste*

[2] *École Normale Supérieure, Paris*

[3] *Universite Pierre et Marie Curie*

[4] *University of Warsaw*

[5] *Brookhaven National Laboratory*

Corresponding Author: laura.foini@gmail.com

In Gibbs equilibrium, fluctuation-dissipation relations can be generically used to probe the thermal properties of the system and measure its temperature.
When the system under study is integrable, though, the dynamics fails to approach such a Gibbs state, reaching instead a generalized ensemble with a macroscopic number of temperature-like parameters which enforce the value of the underlying conserved quantities.
In this setting we show that generalized fluctuation-dissipation relations for appropriately chosen – yet very physical – observables, can be used to infer such temperatures allowing us to reconstruct the non-thermal state.
These results can be applied to a large variety of models including the one dimensional Bose gas where the relevant correlation function is provided by the structure factor, a quantity that can be experimentally accessed.

Session 2 / 26

Time-dependent fluctuations and superdiffusivity in the driven lattice Lorentz gas

Author: Thomas Franosch[1]

Co-author: Sebastian Leitmann [2]

[1] *Universität Innsbruck*

[2] *UIBK Innsbruck*

Corresponding Author: thomas.franosch@uibk.ac.at

We consider a tracer particle on a lattice in the presence of immobile obstacles. Starting from equilibrium, a force pulling on the particle is switched on, driving the system to a new stationary state. We solve for the complete transient dynamics of the fluctuations of the tracer position along the direction of the force. The analytic result, exact in first order of the obstacle density and for arbitrarily strong driving, is compared to stochastic simulations. Upon strong driving, the fluctuations grow superdiffusively for intermediate times; however, they always become diffusive in the stationary state. The diffusion constant is nonanalytic for small driving and is enhanced by orders of magnitude by increasing the force.

Session 6 / **166**

Memory in stochastic and chaotic processes

Author: Andrzej Fulinski[1]

[1] *M. Smoluchowski Institute of Physics, Jagiellonian University, Łojasiewicza 11, Kraków, Poland Polish Academy of Arts & Sciences, Sławkowska 17, 31-016 Kraków, Poland*

Corresponding Author: andrzej.fulinski@uj.edu.pl

Detection and quantification of presence of memory in various stochastic and chaotic processes is discussed. Short introduction of definitions, signatures, and measures is presented, and several examples of the application of the introduced formalism are discussed in detail.

These examples show that nonmarkovian are: most of proceses with stationary correlation function $C(t,s) = C(|t-s|)$ (with notable exception of stationary Ornstein-Uhlenbeck process), chemical reaction, fractional Brownian motions, chaotic processes from Feigenbaum cascade, and quantum processes interacting with heat bath. The discussed methods can be applied also to experimental data in the form of sample paths. It is shown in this way that nonmarkovian are, among others, the driven transport through nanochannels, and Brownian motions of nanoparticles inside living cells.

Session 5 / **108**

Path integral formalism of quantum thermodynamics

Author: Ken Funo[1]

[1] *Peking University*

Corresponding Author: funo1920@tc5.so-net.ne.jp

Path integral formalism of quantum mechanics and quantum field theory has greatly influenced the theoretical developments of physics. For example, a path integral description of open quantum systems has been

used to study the dissipative dynamics of the quantum systems, known as the Caldeira-Leggett model of the quantum Brownian motion. Studies of thermodynamics in the dissipative quantum systems have attracted renewed interest quite recently, owing to the experimental verification of the nonequilibrium equalities and the experimental implementation of quantum information heat engines.

In this presentation, we develop a formalism for quantum thermodynamics based on path integral methods. This may give new insights and understandings about the work and heat in quantum systems. In doing so, we use the Caldeira-Leggett model and study the work and heat statistics. This allows us to study the non-Markov, non-rotating wave, strong coupling regime without making any approximations. Using the path integral method, we have derived the quantum work and heat functionals depending on the path integral trajectories of the system. Taking the semi-classical limit, we proved analytically the convergence of the work and heat functionals (and thus their statistics) to their classical counterparts.

Session 2 / **74**

A tribute to Marian Smoluchowski's legacy on colloid type matter aggregation, and related issues

Author: Adam Gadomski[1]

Co-author: Marcel Ausloos [2]

[1] *UTP University of Science and Technology Bydgoszcz, Poland*

[2] *GRAPES, Liège, Belgium & University of Leicester, UK*

Corresponding Author: agad@utp.edu.pl

In 1916 Marian Smoluchowski proposed a case of constant-kernel cluster cluster aggregation, for which it is manageable to find analitycally by employing scaling arguments, a solution in terms of the cluster size (k) distribution function, n(k) [1,2].
By applying this scaling function it is then possible to get, within the long times' limit, the results for the mean cluster size {k} and the total number of the clusters N, both scalable in terms of time t with a single exponent, g [2].
The clustering arguments, first introduced by Smoluchowski [1], are easily applicable to statistical description of physical-metallurgical processes and ceramic-polycrystalline evolutions, termed the normal grain growth, in which bigger clusters grow at the expense of their smaller neighboring counterparts due to capillary conditions [3].
The normal grain growth, and its dynamics, can be expressed in d-dimensional space (d - Euclidean dimension of the space). Upon identifying {k} from the Smoluchowski description with {R}, the mean cluster radius' size from the normal grain growth approach, and by taking the "extreme" condition of k » 0, one is able to embark on their equivalence by stating rigorously that g=1/(d+1), since the asymptotic scaling rule for N (here: the number of grains) goes via a simple logarithmic depiction as: ln[N]~-ln[g].
The crucial assumption, however, that assures the equivalence claimed, appears to be fully feasible when rearranging the time domain by substituting t in a way such that a new rescaled time variable T(t) is given by a definite integral in [0,t] upon dT(t)=dt/f(t), with an adjustable function f, coming from the dispersive or long-tail, or fractal kinetics' arguments [4].
The arguments may at least qualitatively concern biomembranes dynamics; they can also contribute to nucleation-growth processes in (psychodynamic-clustering) living matter conditions [5-7].

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Session 9 / **3**

Random dynamics in a trap: killing vs survival

Author: Piotr Garbaczewski[1]

[1] *University of Opole*

Corresponding Author: pgar@uni.opole.pl

We consider the random dynamics in a bounded domain, while concentrating on somewhat unexplored links between the absorbing and inaccessible boundarz data impact upon random motion. Both Brownian and Levy-stable dynamics will be discussed , with a focus on tyhe long term surival, and the permanent trapping scenarios.

Session 6 / **88**

Complex dynamics of genomic sites in the nucleus of live cells

Author: Yuval Garini[1]

[1] *Bar Ilan University*

Corresponding Author: yuval.garini@biu.ac.il

The DNA in a human cell is ~3 meters long. It is dynamic and yet is well organized. What are the mechanisms that organizes the chromatin and chromosomes in the nucleus?

Using dynamic methods in live cells, we identified a mechanism that maintains the genome organization in the nucleus. We claim that lamin A forms chromatin loops by lamin A dimers (or oligomers) thereby restricting the chromatin dynamics significantly. This can explain the maintenance of chromosome territories in the nucleus.

We use advanced methods for studying the dynamics of chromatin and proteins in the nucleus. These methods are based on measuring the signal and fluctuations of fluorescent molecules and the use of biophysical models based on Smoluchowski equation and modified diffusion equations. It allowed us to identify that ~50% of a crucial protein named lamin A is bound to the chromatin everywhere in the nucleus interior.

Specific sites along the chromatin commonly exhibit anomalous diffusion (alpha in the range of 0.4-0.7). When lamin A is eliminated, the diffusion dramatically changes to normal diffusion, which is difficult to understand. By analyzing the diffusion in specific time-windows, we show that the dynamics of the genomic sites is bimodal; they are normally constrained and exhibit anomalous diffusion, except for short time-windows where they super-diffuse.

By using single-molecule methods including tethered particle motion (TPM) and atomic force microscopy (AFM) we show the type of bonds formed by lamin A and demonstrate the actual bonding that lamin A forms on the DNA.

Session 13 / **57**

Microreversibility, current fluctuations, and entropy production in nonequilibrium systems

Author: Pierre Gaspard[1]

[1] *Universite Libre de Bruxelles (U.L.B.)*

Corresponding Author: gaspard@ulb.ac.be

On the basis of microreversibility, fluctuation relations are established for the counting statistics of coupled currents flowing across classical or quantum systems sustaining nonequilibrium steady states. Thanks to these relations, the Green-Kubo formulae and the Casimir-Onsager reciprocity relations can be generalized from linear to nonlinear response properties. These advances provide a framework to formulate nonequilibrium thermodynamics in small systems. In this framework, the entropy production can be interpreted as the order parameter of time-reversal symmetry breaking at the statistical level of description. These results apply to hydrodynamic flows, driven Brownian motion, active particles, molecular motors, polymerizations, reactions, as well as to quantum transport in mesoscopic devices.

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Session 8 / **90**

Lyapunov spectral analysis of randomly coupled systems

Author: Anandamohan Ghosh[1]

[1] *Indian Institute of Science Education and Research Kolkata*

Corresponding Author: anandamohan@iiserkol.ac.in

The collective dynamics of coupled units arranged on a random network exhibits complex dynamics ranging from synchronization to spatio-temporal chaos. It is often important to identify if perturbations spread across the network or are confined locally, in
the presence of quenched disorder. The spectrum of Lyapunov exponents, quantifying the sensitivity to perturbations, can be analyzed analogously to the spectrum of eigenvalues of a random matrix.

Simple tools of Random Matrix Theory applied to the Lyapunov spectrum reveal universal features and localization properties emergent from classical deterministic dynamics.

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Session 6 / **91**

Generalized Poisson-Kac processes in statistical physics, thermodynamics and transport

Author: Massimiliano Giona[1]

[1] *University of Rome La Sapienza DICMA*

Corresponding Author: massimiliano.giona@uniroma1.it

Langevin equations driven by vector-valued Wiener noise represent the prototypical model of evolution equations for a physical system driven by a deterministic velocity field in the presence of superimposed stochastic fluctuations. The statistical nature of a Wiener process can be regarded as the natural legacy of a large number ansatz, in which the effects of many unknown and uncorrelated perturbations justifies the Gaussian nature for the increments of the stochastic forcing. Analogously, in dealing with stochastic field equations (stochastic partial differential equations), $\partial\phi(\mathbf{x},t)/\partial t = \mathcal{N}[\phi(\mathbf{x},t)] + a(\phi(\mathbf{x},t))\, f_s(\mathbf{x},t)$, the most common assumption for the stochastic spatio-temporal forcing $f_s(\mathbf{x},t)$ is its delta-correlated nature in space and time ("derivative of a Wiener process").

Notwithstanding the analytical advantages, the assumption of stochastic perturbation of Wiener nature entails some intrinsic shortcomings. The most striking one is the unbounded speed of propagation of stochastic perturbations that, at a microscopic level, is one-to-one with the fractal nature (almost nowhere differentiability) of the graph of a generic realization of a Wiener process. The resolution of the infinite propagation velocity problem has been proposed by C. Cattaneo in the form of a hyperbolic diffusion equation, now bearing his name. In 1974 M. Kac provided a simple stochastic model, for which the associated probability density function is a solution of the Cattaneo equation. In point of fact, it is well known that the Cattaneo model in spatial dimension higher than one does not admit any stochastic interpretation and that the solutions of the Cattaneo model do not preserve positivity.

In order to overcome this problem and to provide a stochastic background to the extended thermodynamic

theories of irreversible phenomena, the original
Kac model has been recently extended and generalized in any spatial dimension
via the concept of Generalized Poisson-Kac (GPK) processes.
In this presentation, after a brief review of GPK theory
we discuss some new results and applications
in statistical physics.

Specifically:

(i) Motivated by the title of the present conference
"On the Uniformity of Laws of Nature", it is addressed
how Poisson-Kac and GPK processes permit to resolve the
"singularities" in the solutions of classical
parabolic transport equations. This is not only related to the
resolution of the paradox of infinite propagation velocity,
but involves also the description of boundary-layer dynamics and the
group properties of the associated Markov operator.

(ii) The latter issue is closely related to the
intrinsic "spinorial" statistical description
of GPK processes, that naturally emerges from the relativistic
description of stochastic kinematics.

(iii) It is addressed how the application
of GPK fluctuations in stochastic partial differential
equation ensures the preservation of positivity of the
field variable (if required by physical principles, for instance
whenever $\phi(\mathbf{x}, t)$ represents a concentration)
and avoids the occurrence of
diverging correlation function, problem that arises
even in the
simplest (linear) stochastic partial differential equations
in the presence of delta-correlated noise fields.
The most striking example is the Edwards-Wilkinson model in
spatial dimensions higher than one.

(iv) Finally, the application of GPK is addressed in connection
with the modeling of systems of interacting particles.

Session 9 / **12**

Dynamics of self-propelled colloidal particles in viscoelastic fluids

Author: Juan Ruben Gomez Solano[1]

[1] *Universitaet Stuttgart*

Corresponding Author: r.gomez@physik.uni-stuttgart.de

The motion of many natural microswimmers, e.g. bacteria and spermatozoa, commonly takes place in viscoelastic fluids and under confinement close to solid walls. The understanding of their swimming mechanisms has triggered a lot of experimental and theoretical work in recent years as well as the development of self-propelled colloidal particles. Although the motion of such synthetic microswimmers in Newtonian fluids has been extensively studied, and they are nowadays a paradigm in non-equilibrium soft matter [1], so far only few investigations have focused on the swimming of microorganisms in viscoelastic fluids [2]. In our work, we experimentally investigate the dynamics of spherical colloidal microswimmers in viscoelastic fluids, which are self-propelled by local demixing of a critical binary polymer mixture induced by laser illumination. Unlike the motion in Newtonian

liquids, we observe a pronounced enhancement of rotational diffusion with increasing particle velocity [3], thereby revealing an unexpected breakdown of the Stokes-Einstein relation for the particle orientation. We demonstrate that this non-equilibrium effect originates from the coupling between the directed particle motion, and the slow microstructural relaxation of the surrounding fluid [4]. Furthermore, we show that such a coupling gives rise to a wealth of new non-equilibrium phenomena with no counterpart in Newtonian liquids, e.g. for the particle translational and rotational dynamics close to solid walls, as well as for collective motion in crowded environments.

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Session 12 / **150**

Operational method for fractional Fokker-Planck equation

Author: Katarzyna Gorska[1]

[1] *Institute of Nuclear Physics, Polish Academy of Sciences*

Corresponding Author: k.gorska80@gmail.com

I will present the results for fractional equations of Fokker-Planck type using evolution operator method. I will employ exact forms of one-sided Levy stable distributions to generate a set of self-reproducing solutions. Explicit cases are reported and studied for various fractional order of derivatives, different initial conditions, and for different versions of Fokker-Planck operators.

Session 2 / **8**

Stationary diffusion among partially reactive sinks: from von Smoluchowski to recent advances

Author: Denis Grebenkov[1]

Co-author: Sergey Traytak [2]

[1] *CNRS*

[2] *Semenov Institute of Chemical Physics of the Russian Academy of Sciences*

Corresponding Author: denis.grebenkov@polytechnique.edu

In 1917, von Smoluchowski founded the first mathematical theory of diffusion-limited reactions by computing the diffusive flux towards a perfect spherical sink. In spite of many advances over the past hundred years, stationary diffusion in complex media with numerous sinks of various shapes and reactivities remains poorly understood. After a brief overview, we present a recently developed generalized method of separation of variables (GMSV) to solve boundary value problems for the Poisson equation in three-dimensional canonical domains (e.g., parallelepipeds, cylinders, spheres, spheroids, ...,

and their combinations). In particular, we derive a semi-analytical representation of the Green function for an arbitrary configuration of non-overlapping partially reactive spherical sinks. This is the key object to determine various characteristics of stationary diffusion such as reaction rate, escape probability, harmonic measure, residence time, and mean first passage time, to name but a few. Based on this solution, we introduce and investigate an effective reaction radius of individual sinks or their clusters that significantly generalizes the famous Smoluchowski formula by accounting for diffusion interactions between sinks and their mutual screening.

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What drives transient behaviour in complex systems?

Author: Jacek Grela[1]

[1] *LPTMS, Universite Paris-Sud*

Corresponding Author: jacekgrela@gmail.com

We study transient behaviour in the dynamics of complex systems described by a set of non-linear ODE's. Destabilizing nature of transient trajectories is discussed and its connection with the eigenvalue-based linearization procedure. The complexity is realized as a random matrix drawn from a modified May-Wigner model. Based on the initial response of the system, we identify a novel stable-transient regime. We calculate exact abundances of typical and extreme transient trajectories finding both Gaussian and Tracy-Widom distributions known in extreme value statistics. We identify degrees of freedom driving transient behaviour as connected to the eigenvectors and encoded in a non-orthogonality matrix T_0. We accordingly extend the May-Wigner model to contain a phase with typical transient trajectories present. An exact norm of the trajectory is obtained in the vanishing T_0 limit where it describes a normal matrix.

Based on:

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Session 7 / **180**

Some analytical methods of solutions to nonlinear diffusion equation

Author: Zbigniew Grzywna[1]

Co-author: Przemyslaw Borys [1]

[1] *Silesian University of Technology, Faculty of Chemistry*

Corresponding Author: zbigniew.grzywna@polsl.pl

From a reach family of nonlinear diffusion equations the Burgers' and Porous Medium equations have been chosen to demonstrate the possibility of getting their analytical solutions of some practically important IBVs problems. A comparison between numerical and analytical solutions have also been provided.

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Continuous-time random walk with multi-step memory: an application to market dynamic

Author: Tomasz Gubiec[1]

Co-author: Ryszard Kutner [1]

[1] *University of Warsaw*

Corresponding Author: tomasz.gubiec@fuw.edu.pl

An extended version of the Continuous-Time Random Walk (CTRW) model with memory is herein developed [1,2].
This memory involves the dependence between arbitrary number of successive jumps of the process while waiting times between jumps are considered as i.i.d. random variables.
This dependence was established analyzing of empirical histograms for the stochastic process of a single share price on a market within the high frequency time scale.
Then, it was justified theoretically by considering bid-ask bounce mechanism containing some delay characteristic for any double-auction market.
Our model appeared exactly analytically solvable.
Therefore, it enables a direct comparison of its predictions with their empirical counterparts, for instance, with empirical velocity autocorrelation function.
Thus, the present research significantly extends capabilities of the CTRW formalism.

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Nonequilibrium Kosterlitz-Thouless transition in a three-dimensional driven disordered system

Author: Taiki Haga[1]

[1] *Kyoto University*

Corresponding Author: haga@scphys.kyoto-u.ac.jp

Two dimensional (2D) systems with global $U(1)$ symmetry such as liquid Helium films and superconducting arrays of Josephson junctions exhibit a topologically ordered phase, which is characterized by power-law decay of the correlation function. The transition from such a quasi-long-range order (QLRO) phase to a disordered phase is called the Kosterlitz-Thouless (KT) transition. The peculiarity of this transition comes from the fact that it is caused by the structural changes in topological defects. Since the geometries and interactions of the topological defects crucially depend on the spatial dimensions, it is intriguing to understand the role of spatial dimensionality in the realization of the KT transition. In the first step toward clarifying this problem, we ask whether there exists a topologically ordered phase and a KT transition in higher dimensions.

It is well known that a quenched disorder can significantly change the large-scale physics of phase ordering systems. One might expect the possibility that the disorder leads to a novel type of KT transition. In fact, some 2D disordered systems are known to exhibit a disorder-induced KT transition at zero temperature. However, to the best of our knowledge, there is no example of a higher-dimensional disordered system which exhibits a KT transition in equilibrium.

In this study, we show that the three-dimensional random field XY model exhibits a topologically ordered phase and a KT transition when it is driven at a uniform velocity. In the first part of this

study, we consider the spin-wave model in which the vortices are ignored. By applying the non-perturbative renormalization group approach, we show that the spin-wave model exhibits a QLRO phase, wherein the correlation function shows power-law decay with an exponent that depends on the disorder strength and the driving velocity. This QLRO phase resembles the topologically ordered phase in the 2D pure XY model. In the second part, we develop a phenomenological theory of the KT transition by taking into account the effect of the vortices. The change in the vortex structure at the transition point is also discussed.

Session 3 / **52**

Foundations of the local equilibrium concept

Author: Rudolf Hilfer[1]

[1] *Universitaet Stuttgart*

Corresponding Author: hilfer@icp.uni-stuttgart.de

Local equilibrium states change slowly in time because they are almost stationary. As a consequence local equilibrium states have to be related to local states that are time-invariant. It has been argued in the literature that a proper mathematical formulation of local equilibrium states must start from the class of time-invariant measures for infinitely extended systems [1]. This presentation argues that the set of time-invariant measures of infinite systems is too small [2]. A suitable extension are states of bounded mean oscillation (BMO-states) that are also close to time-invariant states. BMO-states are states for which the expectation values of all observables are functions of bounded mean oscillation in time. Results for long time scaling limits of induced time flows on subsets of BMO-states then provide the mathematical foundation for the local equilibrium concept.

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Session 6 / **6**

Principles of design of artifical and biological molecular engines

Author: Robert Holyst[1]

[1] *Institute of Physical Chemistry PAS*

Corresponding Author: robert.holyst@gmail.com

Molecular engines are based on different principles than macroscopic motors. I will present two examples: artifical engine created in our lab namely nano-wind mill driven by evaporation of water and the motion of kinesin motor walking on microtubules. This biological engine, of incredibly efficiency, is driven by thermal noise, while consumption of ATP is mainly used for detachment of its parts from microtubule. The key principle in its design is the proper synchronization of its diffusion driven by thermal noise with the hydrolysis of ATP, detachment of ADP and further attachement of

ATP, as we show in our experiment. Our nano-wind mill does work due to spatial organization and synchronization of many motors, which in concerto respond to flux of water.

The presentation was supported by the National Science Centre, Poland within the grant Maestro UMO-2016/22/A/ST4/00017.

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Session 5 / **13**

Quantum measurements of work fluctuations

Author: Karen Hovhannisyan[1]

Co-authors: Antonio Acín [2]; Elisa Bäumer [3]; Marcus Huber [4]; Martí Perarnau-Llobet [2]

[1] *Department of Physics and Astronomy, University of Aarhus, DK-8000 Aarhus C, Denmark*

[2] *ICFO-Institut de Ciencies Fotoniques, The Barcelona Institute of Science and Technology, 08860 Castelldefels, Barcelona, Spain*

[3] *Institute for Theoretical Physics, ETH Zurich, 8093 Zürich, Switzerland*

[4] *Institute for Quantum Optics and Quantum Information (IQOQI), Austrian Academy of Sciences, Boltzmanngasse 3, A-1090 Vienna, Austria*

Corresponding Author: karen@phys.au.dk

Work is one of the central notions in (statistical) mechanics and thermodynamics. In fact, it is *the* quantity that connects thermodynamics and mechanics. Unlike in the macroscopic regime, at the microscale, fluctuations of work become relevant and sometimes even dominant, which makes their characterization a question of fundamental importance. In classical mechanics, the solution is straightforward: to each phase-space trajectory, one assigns the value of the work performed along it. In the quantum regime, however, there is no notion of trajectory, and defining fluctuations of work becomes problematic, especially for coherent processes. In this work, we approach the problem in the most general form, and, therefore, consider closed systems and ask whether there exists at all a definition satisfying two minimal conditions: (1) Average work should be given by the difference of initial and final average energies of the system and (2) the classical limit should be respected. Among many possible ways to define the classical limit, we choose arguably the weakest one – the Jarzynski equality must hold for all thermal initial states. First, we prove that the only work measurement scheme satisfying (2) is the widely-used two-projective-energy-measurements (TPEM) scheme, where the energy is measured both at the beginning and at the end of the process. Second, we show that there exists no state-independent measurement protocol that can simultaneously satisfy (1) for all states and coincide with the TPEM scheme for energy-diagonal initial states. Having thus ruled out the possibility of existence of universal, state-independent generalized quantum measurements for work estimation, we go on asking whether there exist state-dependent schemes capable of satisfying both (1) and (2). It turns out that such measurements do exist, and we describe a simple and intuitive scheme based on the notion of *ergotropy* and its fluctuations as given by a time-reversed TPEM scheme.

Session 1 / **37**

(Quantum)-Thermodynamics at strong coupling and its implications for Stochastic Thermodynamics

Author: Peter Hänggi[1]

Co-author: Peter Talkner [1]

[1] *University of Augsburg*

Corresponding Author: hanggi@physik.uni-augsburg.de

The case of strong system-environment coupling plays an increasingly seminal role when it comes to describe systems of small size which are in contact with an environment. The commonly known textbook situation refers solely to a weak coupling situation for which the equilibrium state of the system is described by a Gibbs state. This situation changes drastically, however, when strong coupling is at work; then, the interaction energy can be of the order of the (sub)-system energy of interest [1]. Let us consider first an overall thermal equilibrium of a total setup composed of a system Hamiltonian H_S, coupling Hamiltonian H_{int} and a bath Hamiltonian H_B.

Based on an explicit knowledge of the so termed *Hamiltonian of mean force* [2], the classical statistical mechanics and, as well, the quantum thermodynamics of open systems which are in contact with a thermal environment – at arbitrary strong interaction strength – can be formulated. Yet, even though the Hamiltonian of mean force uniquely determines the thermal phase space probability density (or the density operator, respectively) of a strongly coupled open system, the knowledge of this quantity alone is *insufficient* to determine the Hamiltonian of mean force itself; the latter must be known for constructing an underlying Stochastic Thermodynamics. This fact presents a major stumbling block for any classical Stochastic Thermodynamics scenario which solely builds upon the knowledge of (observed or calculated) open system trajectories. – In the classical case we demonstrate that under the assumption that the Hamiltonian of mean force is known explicitly, an extension of thermodynamic structures from the level of averaged quantities to *fluctuating* objects (such as internal fluctuating energy, heat, entropy, or free energy); i.e., a Stochastic Thermodynamics, is possible. However, such a construction is by far not unique but involves a vast ambiguity.

Generally, however, the situation becomes a No-Go if we consider an initial nonequilibrium where even the concept of a Hamiltonian of mean force does not exist [1, 3].

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Session 8 / **100**

Autonomous thermal motors

Author: Alberto Imparato[1]

[1] *University of Aarhus, Department of Physics and Astronomy*

Corresponding Author: imparato@phys.au.dk

We present a minimal model
of autonomous thermal motor, made of two interacting

Brownian particles, sitting on two periodic potentials, and kept at different temperatures. We show that such a system does not require ratchet potentials (with
, e.g., an asymmetric saw-tooth shape) in order to exhibit direct
transport, but presents a spontaneous symmetry breaking.
Both the dynamic and thermodynamic properties of the model are discussed.
We find that while the model can be solved exactly in the limit of strong coupling between the particles, the optimal operation regime occurs at moderate coupling strength.

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Universal form of stochastic evolution for slow variables in equilibrium systems

Author: Masato Itami[1]

Co-author: Shin-ichi Sasa [1]

[1] *Kyoto University*

Corresponding Author: itami@fukui.kyoto-u.ac.jp

Nonlinear, multiplicative Langevin equations for a complete set of slow variables in equilibrium systems are generally derived on the basis of the separation of time scales. The form of the equations is universal and equivalent to that obtained by Green. An equation with a nonlinear friction term for Brownian motion turns out to be an example of the general results. A key method in our derivation is to use different discretization schemes in a path integral formulation and the corresponding Langevin equation, which also leads to a consistent understanding of apparently different expressions for the path integral in previous studies.

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Virus capsid, diffusion exponent, and Gaussian fluctuation

Author: Yuichi Itto[1]

[1] *Aichi Institute of Technology*

Corresponding Author: itto@aitech.ac.jp

Virus capsid exhibits an exotic diffusion phenomenon in a cell nucleus [1,2]. The distribution of the diffusion exponent takes a universal Gaussian form for two different types of the virus. Here, the statistical property of the local fluctuations of the diffusion exponent over the nucleus is discussed [3]. It is shown that the statistical distribution of the fluctuations derived by an entropic approach [4] is consistent with the Gaussian form. Local areas of interchromatin corrals are regarded as cubic blocks, (following a discussion originally made for a different cell [5]), and it is examined how large the number of blocks is. Based on the fluctuation distribution, a proposition is also presented for the form of the distribution of waiting time that the virus capsid stays in a given block.

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Modeling the ASF (African Swine Fever) spread and risk assessment for Poland

Author: Andrzej Jarynowski[1]

Co-author: Vitaly Belik [2]

[1] *Smoluchowski Institute of Physics, Jagiellonian University*

[2] *Department of Veterinary Medicine, Freie Universitaet Berlin*

Corresponding Author: andrzej.jarynowski@uj.edu.pl

Problem: Recent rapid spread of the African Swine Fever (ASF) in the Northeast Poland during summer 2017 encourages us to prepare risk assessment for the whole country and predict future geographical transmission paths. The disease has been occurring in Poland since February 2014, however, only in 2017 it exceeded the so-called population reproduction number of the epidemic (adjusted epidemic reproduction rate). The time is running and most of Poland is currently at the highest risk of becoming endemic. Although the Polish Veterinary Inspection with and National Research Institutes are monitoring and controlling the disease spread, a mathematical model of the spatial and temporal dynamics of the disease spread is missing.

Aims: We focus on a predictive stochastic ASF model based on empirical geographical data incorporating organizational network of regions, empirical forest, swine, and wild boar density theoretical organizational structure of the pork production supply chain. This model would be equipped with decision support systems as a tool for epidemiologists. In the preliminary setup, we perform early epidemic growth estimation and simulate landscape-based propagation.

Methods and Data: The early growth estimation can be easily done by matching incidence trajectory to the exponential function, resulting in the approximation of the force of infection. With these calculations the basic reproduction rate of the epidemic, the effective outbreaks detection and elimination times could be estimated. In the spatial model we use forest coverage, pig population in poviats and the distance between centroids of poviats. We use pseudo-gravitational models of short and long-range interactions referring to the socio-migratory behavior of wild boars and the pork production chain. We estimate the model parameters specific for Poland, using a prior Russian and Ukrainian data on ASF spread.

Results and Preliminary Conclusions: Early epidemic growth estimation indicates that to keep the epidemiological status quo will require a very fast response from veterinary services (less than one week after detection to eliminate a single outbreak). Spatial modeling in a certain range of parameters proves the existence of a natural protective barrier within boarders of the 'Congress Poland'. The spread of the disease to the 'Greater Poland' should result in the accelerated outbreak of ASF.

Session 13 / **124**

Guessing the direction of Time's Arrow: theory and experiment

Author: Christopher Jarzynski[1]

[1] *University of Maryland, College Park*

Corresponding Author: cjarzyns@umd.edu

As famously articulated by Sir Arthur Eddington, the second law of thermodynamics implies a directionality to the flow of time: the arrow of time points in the direction of increasing entropy. This deep fact of Nature is something that we intuitively grasp in our everyday lives, which is why we typically find it easy to distinguish between a movie played forward in time, and one played backward. With nanoscale systems the situation becomes more subtle due to the prominence of statistical fluctuations. At sufficiently small length and time scales, a system may behave in a manner that appears contrary to the second law. Surprisingly, our ability to distinguish the direction of the arrow of time can be quantified and shown to obey a universal law. I will show how this law emerges from non-equilibrium fluctuation relations, and I will present experimental results that have verified its validity, using a driven quantum dot.

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Multipartite entanglement of X-matrices in Davies environment

Author: Konrad Jałowiecki[1]

Co-author: Jerzy Dajka [1]

[1] *Institute of Physics, University of Silesia in Katowice, Katowice, Poland*

Corresponding Author: konrad.jalowiecki@smcebi.edu.pl

We consider time evolution of genuinely multipartite entangled N-qubit states initially prepared in the form of X-matrices.
In the scenario that we analyse, one qubit of the considered system is coupled to the thermal environment modelled using the rigorous
Davies theory. We present analytical formulae for the genuinely multipartite concurrence in such system as a function of time both in
scenario with and without energy dissipation. In particular, we analyse the neccessary and sufficient conditions for presence of so
called entanglement sudden death phenomenon.

Session 6 / **140**

Deep learning – results, origin and relation to statistical physics

Author: Czeslaw Jedrzejek[1]

[1] *Poznan University of Technology*

Corresponding Author: czeslaw.jedrzejek@put.poznan.pl

Machine learning (ML), a fundamental concept of AI research, has recently been dominated by advanced statistical techniques (known as deep learning). The origin the methods comes from network optimization and prior knowledge of brain with serious physics inputs. The progress in theoretical architectural models (such as Recurrent Neural Networks (RNN, Convolutional Neural Networks, Long Short-Term Memory networks (LSTM) and Deep Boltzmann Machines) as well as numerical methods make advanced NN to approximate arbitrary functions better than traditional ML methods given sufficiently large amounts of data. A list of cognitive tasks that deep learning systems beat humans grows monthly. This fact changes the way society operates technologically. Among others, instead of coding (i.e. entitling computers with rules) it would be more effective to teach a system

providing data.
The examples of applications mainly from Natural Language Processing and understanding area will be given. Increasingly larger number of companies are bringing to market innovative, smart products and services using AI. Search, mapping genotype to phenotype, advanced medical diagnosis and testing and drug creation are one of the most promising applications. Further progress will be achieved by using knowledge from reverse engineered brain functions.

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Higher-order interactions in human chromosomes: finding topologically associated domains via network community detection

Author: Sang Hoon Lee[1]

Co-authors: JAE HYUNG Jeon [2]; Ludvig Lizana [3]

[1] *Korea Institute for Advanced Study*

[2] *Department of Physics, Pohang University of Science and Technology(POSTECH)*

[3] *Umeå University*

Corresponding Authors: jeonjh@postech.ac.kr, ludvig.lizana@umu.se, lshlj82@kias.re.kr

In this post-genome sequence era, the investigation of the genomic interactions on top of the identified sequence is of great importance. There exist nontrivial structural properties in the interactions, despite the fact that the sequence itself is a topologically simple one-dimensional structure. In particular, topologically associated domains (TADs), representing the group or modular structures, are crucial substructures of chromosome interactions. As the weighted network structures effectively capture the genomic interactions, the identification of TADs naturally corresponds to finding the modular or community structures in the genomic interaction network. In this work, we suggest a systematic way to identify TADs using network community identification algorithms. As a concrete example, we take a representative genomic interaction data called the Hi-C map and apply algorithms for network community detection, in particular, with the tunable resolutions parameter that enables us to find TADs with various resolutions. For validity of our method, we compare several known biological markers for the TAD boundary, such as the enrichment of transcriptional repressor CTCF, with our systematically identified TADs

Session 4 / **142**

Aging transient superdiffusive dynamics in in vivo neuronal mRNP transport: a Levy walk description

Authors: Heyoon Park[1]; Hyungseok Moon[1]; Jae Hyung Jeon[2]; Minho Song[1]

[1] *Seoul National University*

[2] *Department of Physics, Pohang University of Science and Technology(POSTECH)*

Corresponding Author: jeonjh@postech.ac.kr

Localization of messenger ribonucleoproteins (mRNPs) plays an essential role in the regulation of gene expression required for long-term memory formation and neuronal development. Knowledge concerning the nature of neuronal mRNP transport is thus crucial for understanding how mRNPs are delivered to their target synapses. In this talk, we show experimental and theoretical evidence that the active transport dynamics of neuronal mRNPs, which is distinct from the previously reported motor-driven transport, follows an aging Levy walk. Such nonergodic, transient superdiffusion occurs because of two competing dynamic phases: the motor-involved ballistic run and static localization of mRNPs. Our proposed Levy walk model reproduces the experimentally extracted key

dynamic characteristics of mRNPs with quantitative accuracy. Moreover, the aging status of the mRNP particles in an experiment is inferred from the model. The potential physical mechanisms for the observed aging behaviors are shortly discussed.

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Low density lipoproteins (LDL) accumulation in right coronary artery

Author: Katarzyna Jesionek[1]

Co-author: Marcin Kostur [1]

[1] *Institute of Physics, University of Silesia, 40-007 Katowice, Poland and Silesian Center for Education and Interdisciplinary Research, University of Silesia, 41-500 Chorzow, Poland*

Corresponding Author: katarzyna.jesionek@smcebi.edu.pl

The convection-diffusion-reaction equation can be used to model the transport of the low-density lipoproteins (LDL) in the
arterial wall. LDL is a lipoprotein associated with the development of the atherosclerotic plaque and coronary artery disease. In this poster we present LDL concentration profiles obtained for patient specific right coronary artery. The case with normal pressure
and hypertension are discussed. Simulations of the LDL concentration based on medical imaging may become an important diagnostic tool. Simulation results indicate points, where atherosclerosis may occur.

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Stochastic gene expression in cells undergoing division

Author: Jakub Jędrak[1]

Co-author: Anna Ochab-Marcinek [2]

[1] *Instytut Chemii Fizycznej PAN, ul. Kasprzaka 44/52, 01-224 Warszawa*

[2] *Institute of Physical Chemistry, Polish Academy of Sciences*

Corresponding Author: jakub.s.jedrak@gmail.com

Stochasticity in gene expression is one of the most important problems of quantitative biology. It has been shown that, in the systems as small as living cells, production of proteins is strongly affected by random fluctuations coming from various sources. As a result, the biological noise is a meaningful factor influencing cellular processes and cell-fate decisions. The particular questions explored within the field of quantitative biology are, among others, the correct identification of noise sources and correct estimation of noise parameters, e.g., frequencies and sizes of the random bursts of protein production.

We propose a stochastic model of gene expression in cells undergoing division. The model combines a deterministic approximation of protein degradation and the two sources of noise: 1) Random bursts of protein production, and 2) more or less random duration of the cell cycle. Random partitioning of proteins between daughter cells is also possible as the third source of noise.

In the classical model proposed by the Xie group, the effect of cell division was tacitly identified with the effect protein degradation. We show that this may not be a correct assumption and the values of mean burst size and mean burst frequency inferred from the experiments using the classical model may be wrong. We show that our model provides more reasonable estimates for these quantities. Moreover, our model demonstrates that the “noise floor”, observed in the experiments and previously

ascribed to an unidentified extrinsic noise, may be the effect of cell division. Our model sets physical constraints, based on the degree of randomness in cell cycle duration, for the levels of noise in gene expression.

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Pair approximation for the q-voter model with independence on complex networks

Author: Arkadiusz Jędrzejewski[1]

[1] *Department of Theoretical Physics, Faculty of Fundamental Problems of Technology, Wrocław University of Science and Technology*

Corresponding Author: arkadiusz.jedrzejewski@pwr.edu.pl

We investigate the q-voter model with stochastic noise arising from independence on complex networks. Using the pair approximation, we provide a comprehensive, mathematical description of its behavior and derive a formula for the critical point. The analytical results are validated by carrying out Monte Carlo experiments. The pair approximation prediction exhibits substantial agreement with simulations, especially for networks with weak clustering and large average degree. Nonetheless, for the average degree close to q, some discrepancies originate. It is the first time we are aware of that the presented approach has been applied to the nonlinear voter dynamics with noise. Up till now, the analytical results have been obtained only for a complete graph. We show that in the limiting case the prediction of pair approximation coincides with the known solution on a fully connected network.

Session 3 / **162**

Long range correlations in dynamical systems and in observed data

Author: Holger Kantz[1]

Co-authors: Katja Polotzek [1]; Marc Hoell [1]; Mozhdeh Massah [1]

[1] *Max Planck Institute for the Physics of Complex Systems*

Corresponding Author: kantz@pks.mpg.de

Long range temporal correlations (LRC)
in noise-like signals can be detected through
the scaling behaviour of the mean squared displacement (MSD) of the pathes
which one obtains by integrating over the signal. Detrended fluctuation
analysis has become a standard tool which beyond a simple MSD analysis is able
to remove the effects of trends on the signal. In the first part of this talk
we present a sketch of theoretical considerations which give a better
justification for DFA than it has been presented before. In the second part,
we show the consequences of LRC on the convergence of time averages, on the
probability for large deviations, and for the estimation of trends. In order
to transfer these findings to real world data, we need paradigmatic data
models with a minimum of free parameters.

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Phase behaviour of monolayers composed of flexible, trimer-like molecules

Authors: Lech Longa[1]; Michał Cieśla[1]; Paweł Karbowniczek[2]

[1] *M. Smoluchowski Institute of Physics, Jagiellonian University, Kraków, Poland*

[2] *Institute of Physics, Cracow University of Technology, Kraków, Poland*

Corresponding Author: pkarbowniczek@pk.edu.pl

Using Onsager-type of Density Functional Theory and constant pressure MC simulations we study the effect of conformational degrees of freedom on orientational and positional ordering of trimer-like molecules confined to monolayers.

The molecules are composed of three linked line segments. Each of the terminal segments is allowed to occupy one of the two internal states: α and -α, where α is an angle between the central and the terminal segment. Depending on the internal state of its terminal segments this flexible hard-needle can dynamically adopt either a chiral zigzag or achiral bow-shaped conformation. A system composed of such molecules has a rich spectrum of stable, liquid-crystalline structures. The Density Functional Theory admits
the existence of nematic and lamellar nonchiral and chiral phases, while Monte Carlo simulation also suggest existence of more complex, modulated structures, with splay-bend
signature. The model is a generalization of recent studies [1-3], where separately zigzag and/or bow-shaped hard-needles were considered.

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Modulated phases in two-dimensional systems of bent-core particles

Authors: Agnieszka Chrzanowska[1]; Lech Longa[2]; Michał Cieśla[2]; Paweł Karbowniczek[1]

[1] *Institute of Physics, Cracow University of Technology, Poland*

[2] *M. Smoluchowski Institute of Physics, Jagiellonian University, Kraków, Poland*

Corresponding Author: pkarbowniczek@pk.edu.pl

We study the role of excluded-volume effects for the stabilization of different phases in systems composed of hard bent-core particles placed on a planar surface. In particular, we analyze molecular systems, in which modulated phases can appear. By the use of combined theoretical and simulational approaches, such as Onsager's Density Functional Theory and Monte Carlo simulations, we investigate how the details of bent-core particles composed of needles, polygons and disks can affect stability of surface order. We start by analyzing bent-core particles with two arms, for which we identified the nematic splay-bend phase, which turned out to be more stable than two-dimensional smectic ordering for particles with large opening angles and thin arms. Then, we present results for

particles with three arms, for which we also identified modulated phases for wide range of molecular parameters. Lastly, we discuss the possibility of existence of nematic splay-bend in systems of banana-shaped molecules composed of connected disks.

This work was supported by Grant No. DEC-2013/11/B/ST3/04247 of the National Science Centre in Poland.

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Session 7 / **141**

Stochastic modeling of diffusion in dynamical systems: three examples

Author: Rainer Klages[1]

[1] *Queen Mary University of London*

Corresponding Author: r.klages@qmul.ac.uk

Consider equations of motion that generate dispersion of an ensemble of particles. For a given dynamical system an interesting problem is not only what type of diffusion is generated by its equations of motion but also whether the resulting diffusive dynamics can be reproduced by some known stochastic model. I will discuss three examples of dynamical systems generating different types of diffusive transport: The first model is fully deterministic but non-chaotic by displaying a whole range of normal and anomalous diffusion under variation of a single control parameter [1]. The second model is a dissipative version of the paradigmatic standard map. Weakly perturbing it by noise generates subdiffusion due to particles hopping between multiple attractors [2]. The third model randomly mixes in time chaotic dynamics generating normal diffusive spreading with non-chaotic motion where all particles localize. Varying a control parameter the mixed system exhibits a transition characterised by subdiffusion. In all three cases I will show successes, failures and pitfalls if one tries
to reproduce the resulting diffusive dynamics by using simple stochastic models.

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Session 12 / **50**

Coordination games on networks

Author: Adam Kleczkowski[1]

Co-authors: Michael Redenti [1]; Nicholas Hanley [2]

[1] *University of Stirling, Scotland*

[2] *University of St Andrews, Scotland*

Corresponding Author: ak@maths.stir.ac.uk

One of the key contributions of Marian Smoluchowski was to show that even small, apparently random, contributions from individuals can combine to produce significant shifts in the collective behaviour. This paradigm is not limited to physics but has become increasingly influential in biological and social sciences. Models have been developed to describe such diverse systems like the market failure or spread and control of infectious diseases. We present a model that combines game theoretical framework for decision-making process involved in controlling plant infection or pest spread with a network model. We study a repeated cooperation game describing actions of plant nursery managers. We show that although the cooperation strategy is not stable (due to the existence of a risk-dominant strategy), the decay rate non-trivially depends on the initial density of cooperators, on the weight they assign to past events, and whether the decision involves an element of a chance. By considering an agent quantal response learning process, we also study how 'irrationality' of decisions influence potential for collaborative actions. Finally, we show that the network structure also impacts on the emergence of cooperation.

Session 9 / **14**

Switching of wake-mediated interaction caused by blockade effect and collective wake formation

Authors: Oleksandr Kliushnychenko[1]; Sergey Lukyanets[1]

[1] *Institute of Physics, NASU, Kiev, Ukraine*

Corresponding Author: kliushnychenko@iop.kiev.ua

The effect of concentration-dependent switching of the wake-mediated interaction between obstacles in a gas flow of interacting Brownian particles is presented. When increasing bath fraction exceeds half-filling, the interaction between obstacles switches from effective attraction to repulsion or vice-versa, depending on the mutual alignment of obstacles with respect to the gas flow. It is shown that for an ensemble of small and widely separated obstacles the dissipative interaction takes the form of induced dipole-dipole interaction governed by an anisotropic screened Coulomb-like potential. This allows one to give a qualitative picture of the interaction between obstacles and explain switching effect as a result of changes of anisotropy direction. The non-linear blockade effect is shown to be essential near closely located obstacles, that manifests itself in the additional screening of gas flow and generation of a pronounced step-like profile of gas density distribution. It is established that behavior of the magnitude of dissipative effective interaction is, generally, non-monotonic in relation to both the bath fraction and the external driving field. It has characteristic peaks corresponding to the situation when the common density "coat" formed around the obstacles is most pronounced. The possibility of the dissipative pairing effect and the effects of enhanced shock-wave formation of wake profiles under the collective scattering of gas flow on impurities are discussed. All the results are obtained within the classical lattice-gas model.

Session 8 / **40**

Anomalous quantum diffusion of hydrogen atoms in proteins

Author: Gerald Kneller[1]

[1] *University of Orleans / CNRS*

Corresponding Author: gerald.kneller@cnrs.fr

Gerald Kneller

Centre de Biophysique Moléculaire
CNRS/University of Orléans, France

Quasielastic neutron scattering (QENS) from biomolecular systems, such as proteins, probes essentially the diffusive single particle dynamics of the hydrogen atoms. As far as the internal dynamics is considered, the motion of the hydrogen atoms exhibits both multiscale and quantum properties. Starting from the definition for the mean square displacement of a quantum particle, it will be shown how both aspects can be combined within a theory of QENS experiments, which is asymptotically exact for long times/low frequencies and for moderate momentum transfers.

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Session 9 / **23**

Subdiffusion in a system consisting of two different media

Author: Tadeusz Kosztolowicz[1]

Co-author: Katarzyna Lewandowska [2]

[1] *Institute of Physics, Jan Kochanowski University in Kielce*

[2] *Medical University of Gdansk*

Corresponding Author: tadeusz.kosztolowicz@ujk.edu.pl

We consider subdiffusion in a system which consists of two homogeneous media joined together; subdiffusion parameters can be different in both media [1,2]. We also consider subdiffusion with absorption in a composite system. The application of the theoretical model to describe a real diffusion processes in the considered system is also presented. Confronting the theoretical formulas with the experimental data we estimate subdiffusive parameters of colistin in aqueous agarose solution and we show the subdiffusive character of colistin transport in the gel.

[1] T. Kosztołowicz, Int. J. Heat Mass Transf. 111, 1322 (2017).
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Session 4 / **34**

Nonergodic dynamics in the plasma membrane of living cells

Author: Diego Krapf[1]

[1] *Colorado State University*

Corresponding Author: krapf@engr.colostate.edu

Tracking individual proteins on the surface of live mammalian cells reveals complex dynamics involving anomalous diffusion and clustering into nanoscale domains. Theoretical models show that anomalous subdiffusion can be caused by different processes. Here we study the nonergodic dynamics of voltage gated ion channels in human embryonic kidney (HEK) cells and in hippocampal neurons. We perform time series and ensemble analysis of extensive single-molecule tracking. We show that in HEK cells, weak ergodicity breaking is found to be maintained by immobilization events that

take place when the proteins are captured within clathrin-coated pits. However, in hippocampal neurons, ergodicity breaking is caused by transient confinement into nanoclusters with a 230-nm mean diameter. Ergodicity breaking in these cells is manifested in two different ways. First, significant differences are observed between time- and ensemble-averaged mean square displacements. Second, a dynamical functional test unmasks ergodicity breaking at the individual trajectory level.

Session 12 / 25

Spin-glass-like transition in the majority vote model with contrarians

Author: Andrzej Krawiecki[1]

[1] *Faculty of Physics, Warsaw University of Technology*

Corresponding Author: akraw@if.pw.edu.pl

Majority vote model on random graphs and scale-free networks is investigated, in which a fraction p of agents (called contrarians or anticonformists)
follows an antiferromagnetic update rule, i.e., they assume, with
probability governed by a parameter q (0 < q < 1/2), the opinion opposite to that of the majority of their neighbors, while the remaining 1-p fraction of agents follows the usual ferromagnetic update rule assuming, with probability governed by the same parameter q, the opinion in accordance with that of the majority of their neighbors. For p=1 it is shown by Monte Carlo simulations and using the Binder cumulants method that for decreasing q the model undergoes second-order
phase transition from a disordered (paramagnetic) state to a spin-glass-like state,
characterized by a non-zero value of the spin-glass order parameter measuring the overlap of agents' opinions in two replicas of the system, and simultaneously by the magnetization close to zero. Besides, in this state the correlation of the agents' opinions exhibits exponentially decaying oscillations, as expected in the spin-glass phase.
In the case of the model on scale-free networks the critical value of the parameter q weakly depends on the details of the degree distribution. As p is decreased, the critical value of q falls quickly to zero and only the disordered phase is observed. On the other hand, for p close to zero for decreasing q the usual ferromagnetic transition is observed.

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Random sequential adsorption of cubes

Authors: Michał Cieśla[1]; Piotr Kubala[1]

[1] *M. Smoluchowski Institute of Physics, Jagiellonian University, Kraków, Poland*

Corresponding Author: pkua.log@gmail.com

Study of properties of hard objects random packings provide insight into a structure of granular media, soft- and bio-matter as well as heterogeneous or composite materials. Numerical modeling of such packing, reveals rules responsible for different processes occurring in them like for example self-assembly of nanoparticles or glass formation, etc.

One approach to random packings uses random sequential adsorption (RSA) algorithm, which is based upon iterations of the following steps:

- a virtual particle is created. Its position and orientation inside a packing are selected randomly.
- the virtual particle is tested for overlaps with any of the other, previously placed, particles. If no overlap is found, it is placed, holding its position and orientation until the end of simulations. Otherwise, the virtual particle is removed and abandoned.

The packing is called saturated or jammed when no more particles can be added to it.

In this study we focus on three dimensional random packings built of unoriented cubes. Previous works considering two-dimensional random packings of unoriented squares provided, among others, unexpected information about kinetics of RSA.

This work was supported by Grant No. 2016/23/B/ST3/01145 of the National Science Centre in Poland.

Session 12 / **103**

Second order optimization may lead to Lévy walks

Authors: Lukasz Kusmierz[1]; Taro Toyoizumi[1]

[1] *RIKEN Brain Science Institute*

Corresponding Author: nalewkoz@gmail.com

Most living organisms perform two different types of search: a directed search (taxis) and a random search. The former is observed when the environment provides cues to guide the motion towards targets,
whereas the latter may not involve any memory and information processing and can be modeled by ran-
dom walks. There is a large body of experimental results showing that the random walk adopted by many
organisms is described well by Lévy walks, which raises questions about the reasons and underlying mech-
anisms of such a behavior. Here we show that Lévy walks may emerge from a directed gradient based
search, which bridges the gap between the two modes of a search. For a wide range of scenarios our model
reproduces the tail index $\alpha = 1$, in line with previous experimental observations in foraging organ-
isms and
predictions based on optimality considerations for sparse targets. Moreover, the model predicts spe-
cific
relations between features of the search and the curvature of the optimized function, which can be tested
experimentally.

Session 7 / **4**

Two forms of heat transfer via interaction with heat bath

Author: Chulan Kwon[1]

[1] *Myongji University*

Corresponding Author: ckwon58@gmail.com

We consider a classical open system in contact with heat bath via interaction Hamiltonian. We investigate two forms of energy transfer via the change of interaction Hamiltonian, which are interpreted as heats. One is heat dissipation from the system and the other is heat absorption by the heat bath, which are usually expected to be the same. Since the change of interaction Hamiltonian leads to the difference between the two heats, the two are not the same in non-stationary period. In non-equilibrium stationary state, the two are only equal to each other in average and may differ

in probability distribution. We investigate the difference of the forms of heat for toy models and molecular dynamic systems. It will be an interesting question which is a relevant choice of heat used for the first and second laws of thermodynamics. Further study on open quantum systems will be interesting.

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A model for non-Gaussian transport in intracellular media

Author: Yann Lanoiselée[1]

Co-author: Denis Grebenkov [2]

[1] *PMC lab - École Polytechnique*

[2] *CNRS*

Corresponding Author: yann.lanoiselee@polytechnique.edu

Recent progresses in single particle tracking have shown evidences of non-Gaussian distribution of displacements in biological media either near the cellular membrane or inside the cytoskeleton. A similar behavior has also been reported in granular media, turbulent flows, gels, colloidal suspensions. Its emergence in various fields suggests that this is a general feature of diffusion in complex media. A possible interpretation of this phenomenon is that tracers experience a medium with spatio-temporal fluctuations which result in local changes of diffusivity. We propose and investigate an ergodic easily interpretable model, which is based on diffusing diffusivity. Depending on the parameters, the displacement distribution can exhibit either a pure exponential shape, or a Gaussian-like behavior at small displacements with an exponential tail at large displacements, or be reduced to a purely Gaussian one in the Brownian limit. We show that the distribution converges to a Gaussian one slowly, as 1/t. We calculate relevant statistical properties and propose steps to estimate the model parameters from a sufficiently long single trajectory.

Session 7 / **16**

Carnot efficiency is attainable in an irreversible process

Author: Jaesung Lee[1]

Co-author: Hyunggyu Park [1]

[1] *Korea Institute for Advanced Study*

Corresponding Author: jslee@kias.re.kr

In thermodynamics, there exists a conventional belief that “the Carnot efficiency is reachable only when a process is reversible.” However, there is no theorem proving that the Carnot efficiency is impossible in an irreversible process. Here, we show that the Carnot efficiency is attainable in an irreversible process through investigation of the Feynman-Smoluchowski ratchet (FSR). Thus, this finding gives us a new possibility to develop a novel design of thermodynamic engines with high efficiency regardless of the reversibility. Our result also answers the long-standing question of whether the Carnot efficiency is possible in the FSR.

Session 7 / 27

Nonuniversality of heat engine efficiency at maximum power

Author: Sang Hoon Lee[1]

Co-authors: Hyunggyu Park [1]; Jaegon Um [2]

[1] *Korea Institute for Advanced Study*

[2] *Seoul National University*

Corresponding Author: lshlj82@kias.re.kr

We study the efficiency of a quantum dot engine in the condition of the maximum power output. In contrast to the quasi-statically operated Carnot engine whose efficiency reaches the theoretical maximum, recent research on more realistic engines operated in finite time has revealed other classes of efficiency such as the Curzon-Ahlborn efficiency maximizing the power. The linear coefficient of such power-maximizing efficiency as a function of the reservoir temperature ratio has been argued to be universal as $1/2$ under the tight-coupling condition between thermodynamic fluxes. By taking the quantum dot heat engine, however, we show that depending on the constraint posed on the engine, the linear coefficient can be unity, which implies that the efficiency at the maximum power actually approaches the Carnot efficiency in the equilibrium limit. As a result, we dismiss the notion of universal linear coefficient of the efficiency at the maximum power, and discuss the implication of such a result in terms of entropy production and irreversible thermodynamics. We claim that the particular scheme for the linear coefficient of unity is actually more realistic and experimentally realizable, as it corresponds to controlling the gate voltage of the quantum dot, for given temperatures and chemical potentials of the leads connected to the quantum dot.

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Theoretical and experimental determination of a boundary contition at a thin membrane for diffusion

Author: Tadeusz Kosztołowicz[1]

Co-authors: Katarzyna Lewandowska [2]; Sławomi Wąsik [1]

[1] *Institute of Physics, Jan Kochanowski University in Kielce*

[2] *Medical University of Gdansk*

Corresponding Author: kale@gumed.edu.pl

We present a method of deriving a boundary condition for diffusion at a thin membrane from experimental data. Within this method the Laplace transform of a boundary condition is assumed to be in the form

$$\hat{C}_2(0^+,p) = \hat{\Phi}(p)\hat{C}_1(0^-,p) \ ,$$

where $\hat{\Phi}(p)$ is a function to be determined. Next, we find the Laplace transform of some theoretical function containing Φ, which is a relatively easy to measure experimentally. Then, this function is also determined by means of a numerical calculation of the Laplace transform of the experimental data obtained for normal diffusion of ethanol in water in a system with a nephrophan membrane. Finally, comparing both Laplace transforms mentioned above, we find the function Φ. The derived boundary condition at a membrane contains a term with a Riemann-Liouville fractional time derivative

$$\alpha C_2(0^+,t) + \beta \frac{\partial^{1/2}}{\partial t^{1/2}} C_2(0^+,t) = C_1(0^-,t) \ .$$

Such a form of the boundary condition shows that particles transfer through a thin membrane is a "long-memory process." The presented method is an example that an important part of the mathematical model of physical processes may be derived directly from experimental data.

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Resonant tunneling through a finite-width potential barrier in graphene nanoribbons

Author: Rodrigo Lima[1]

Co-author: Alexandro Nascimento [2]

[1] *Universidade Federal de Alagoas*

[2] *Instituto Federal de Educação, Ciência e Tecnologia do Piauí, Parnaíba, PI 64210-260, Brazil*

Corresponding Author: rodrigo@fis.ufal.br

This study aims at presenting the calculate the transmission probabilities of Dirac particles through a graphene nanoribbon (GNR) with a barrier-like potential. Using the Dirac equation with continuity condition for wave functions at the interfaces between regions with and without a potential, it was calculated the mode-dependent transmission probability for both semiconducting and metallic armchair-edge graphene nanoribbons (AGNRs). We verified that the transmission is an oscillating function of the height and width of the barrier for both AGNRs. Finally, we can have verified that, different from those for an infinite sheet of graphene system, the transport properties of AGNRs depends sensitively on their widths and edge details. This study is not only of vital importance for understanding the fundamental physics of the material, but also useful for designing novel devices or developing applications.

Session 0 / **135**

Arrays of coupled two-state oscillators

Author: Katja Lindenberg[1]

Co-authors: Alexandre Rosas [2]; Daniel Escaff [3]; Italo Pinto [2]

[1] *University of California, San Diego*

[2] *Universidade Federal de Paraíba, João Pessoa, Brazil*

[3] *Universidad de Los Andes, Santiago, Chile*

Corresponding Author: klindenberg@ucsd.edu

We discuss synchronization of arrays of coupled two-state stochastic oscillators with additional fluctuations due to finite numbers of units, types and ranges of couplings, memory effects, etc. If time permits we present phase diagrams

Session 6 / **116**

Navigation and target search on human chromosomes

Author: Ludvig Lizana[1]

[1] *Umeå University*

Corresponding Author: ludvig.lizana@umu.se

In living cells, proteins often bind to specific basepair sequences on DNA, such as transcription factor proteins that regulate gene expression, or restriction enzymes that cut the DNA at cleavage sites. These proteins search for targets that are about 10 basepairs long, on a DNA that is a few mega basepairs in bacteria, and billions in humans. This sounds like a needle in a haystack- problem but search times are surprisingly short. For example, in *E. coli* bacteria it takes a few minutes to locate a gene regulatory site, whereas a random search would take up to ten times longer. The common explanation for this, is that proteins combine three dimensional (3D) excursions with one dimensional (1D) diffusion along the DNA, also known as facilitated diffusion.

Combining 3D and 1D search in this way implies that search times depend on the DNA's specific 3D organisation. This has been shown analytically using classical polymer models with known looping probabilities and in simulations. But, how this happens in humans and other eucaryotes where DNA organisation is more complex is an open problem. Theoretically, researchers have been hampered by the lack of knowledge of how eukaryotic DNA is organised, but experimental development of so-called Chromosome Conformation Capture techniques, where state-of-the-art is HiC, have partly remedied this problem. In short, HiC experiments give a genome-wide heat map of physical contact frequencies, or looping probabilities, between all DNA fragments pairs in the cell nucleus down to 1 kilo-basepair resolution.

In our recent work, we have used HiC data as a proxy for the *in-vivo* DNA looping probabilities to model protein search on human chromosomes. By mapping the search onto a network problem, with DNA segments as nodes and physical contacts as links, we calculate the mean-first passage time to all nodes for all human chromosomes. For example, we find that DNA segments that harbour gene starts have small search times and are thus easy to find.

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Self-averaging of random quantum dynamics

Author: Marcin Lobejko[1]

Co-authors: Jerzy Dajka [1]; Jerzy Łuczka [1]

[1] *University of Silesia*

Corresponding Author: mlobejko@us.edu.pl

Stochastic dynamics of a quantum system driven by statistically independent random sudden quenches is studied. We show that with growing frequency of random quenches the system smoothly approaches deterministic limit indicating self-averaging of its temporal evolution. Moreover we reveal

that there is an effective (constant) Hamiltonian generating time evolution of self-averaged system directly related to statistical properties of the stochastic driving.

Session 5 / **59**

Diffusion of a tagged particle in two dimensional elastic networks

Author: Michael Lomholt[1]

[1] *University of Southern Denmark*

Corresponding Author: mlomholt@memphys.sdu.dk

I will discuss the long time asymptotic behavior of a tagged particle in two dimensional systems, where the particles are stuck with their neighbors. This corresponds to single-file diffusion in one dimension, where the mean squared displacement of a particle grows with the square root of time. In two dimensions it turns out that the mean square displacement grows logarithmically. I will show how one can arrive at these results through an approach called harmonization.

Session 2 / **164**

Transient anomalous diffusion in ratchet systems

Author: Jerzy Luczka[1]

Co-authors: Jakub Spiechowicz [1]; Peter Hanggi [2]

[1] *University of Silesia*

[2] *University of Augsburg*

Corresponding Author: jerzy.luczka@us.edu.pl

Anomalous diffusion can be detected in various systems. We show that anomalous diffusion may emerge in a straightforward, one dimensional classical nonequilibrium dynamics of a Brownian particle moving in a ratchet potential and driven by both an unbiased time-periodic force and thermal fluctuations of Gaussian nature. In a tailored parameter regime for which the deterministic counterpart of the system is non-chaotic, the mean square deviation of the Brownian particle coordinate evolves in three following stages: initially as superdiffusion, next as subdiffusion and finally as normal diffusion in the asymptotic long time limit. The lifetimes of superdiffusion and subdiffusion can be controlled by system parameters and can last many many orders longer than characteristic times of the system, thus being comfortably detectable experimentally. The findings are distinct from existing knowledge and suggest reconsideration of generally accepted opinion that anomalies are due to large and rare fluctuations that are characterized by broad distributions with power-law tails.
We explain the underlying mechanism standing behind the emergence of diffusion anomalies and control of their regimes which are related to ergodicity of the system and ultraslow relaxation of the particle velocity towards its non-equilibrium stationary state.

Session 7 / **168**

Evolution of information within sEMG signals in the process of treatment

Author: Lukasz Machura[1]

Co-authors: Michał Nowakowski [2]; Paulina Trybek [1]

[1] *University of Silesia*

[2] *Department of Medical Education, Jagiellonian University Medical College*

Corresponding Author: lukasz.machura@smcebi.edu.pl

Colorectal cancer remains to be one among 5 most common types of cancer found for both men and women. Typically multimodal treatment including surgery, radiation and chemotherapy is applied. The electrical activity of external anal sphincter can serve as a potential source of knowledge of the actual state of the patient. The signals registered by means of the surface electromyography are typically highly complex thus create a challenge for its description. The loss of such complexity is often related with the pathological state. Entropy often serves as one of the nonlinear methods capable to grasp an internal structure of the signal together with the insight into its complexity over a wide range of scales. In this work we would discuss the usefulness of the most common techniques for the description of the loss of information carried out by the biomedical signals.

Session 12 / **73**

Temperature gradient induced solvent coarsening around colloids

Author: Anna Maciolek[1]

Co-authors: Siegfried Dietrich [2]; Sutapa Roy [3]

[1] *ICHF PAN*

[2] *MPI for Intelligent Systems*

[3] *MPI for Intelligent Systems, Stuttgart*

Corresponding Author: amaciolek@ichf.edu.pl

Using mesoscopic numerical simulations and analytical theory we investigate
the coarsening of the solvent structure around a colloidal particle emerging after a
temperature quench of the colloid surface. Qualitative differences in the coarsening mechanisms are found,
depending on the composition of the binary liquid mixture forming the solvent and on the adsorption preferences of the colloid. For an
adsorptionwise neutral colloid, as function of time the phase being next to its surface alternates. This behavior sets in on the scale of the
relaxation time of the solvent and is absent for colloids with
strong adsorption preferences. A Janus colloid, with a small temperature difference between its two hemispheres,
reveals an asymmetric structure formation and surface enrichment around it, even if the solvent is within its one-phase region
and if the temperature of the colloid is above the critical demixing temperature T_c of the solvent.
A comparison between the emerging fluid structures above and below T_c is provided.
Our phenomenological
model turns out to capture recent experimental findings according to which, upon laser
illumination of a Janus colloid and due to the ensuing temperature gradient between its two hemispheres, the surrounding binary liquid mixture
develops a concentration gradient.

Session 4 / **54**

Induced motion of a probe in contact with a nonequilibrium medium

Author: Christian Maes[1]

[1] *KU Leuven*

Corresponding Author: christian.maes@kuleuven.be

We discuss how contact with a nonequilibrium bath can modify the effective dynamics of a probe. In particular, systematic forces may become nongradient; the second fluctuation-dissipation relation can be broken and the noise may be nonGaussian and showing power law distributed jumps.

Session 3 / **42**

Dynamical maps on quantum Orlicz spaces

Author: Wladyslaw Adam Majewski[1]

[1] *The Gdansk University*

Corresponding Author: fizwam@univ.gda.pl

We present a new rigorous approach based on Orlicz spaces for the description of the statistics of large regular statistical systems, both classical and quantum. We emphasize that the presented formalism is applicable to QFT!
The pair of Orlicz spaces we explicitly use are respectively built on the exponential function (for the description of regular observables) and on an entropic type function (for the corresponding states). They form a dual pair (both for classical and quantum systems). This pair $\langle L^{\cosh -1}, L\log(L+1)\rangle$ has the advantage of being general enough to encompass regular observables, and specific enough for the latter Orlicz space to select states with a well-defined entropy function.
Quantum dynamical maps are defined and studied for quantum statistical physics based on Orlicz spaces. We show that even in the most general non-commutative contexts, completely positive Markov maps satisfying a natural Detailed Balance condition, canonically admit an action on a large class of quantum Orlicz spaces. This is achieved by the development of a new interpolation technique, specifically suited to the above context, for extending the action of such maps to the appropriate intermediate spaces of the pair $\langle L^{\infty}, L^{1}\rangle$.

Session 3 / **85**

Glass transition as the consequence of spatially correlated stochastic dynamics

Author: Maciej Majka[1]

[1] *Jagiellonian University*

Corresponding Author: maciej.majka@uj.edu.pl

Despite the decades of intense research, the glass transition, i.e. the extreme rise in the viscosity (by 10^{14} for molecular and 10^{3} for colloidal glasses) of the disordered system as it becomes denser/colder, is far from being fully understood. One important limitation here is the lack of analytically solvable models for the systems with arbitrary interactions. In this presentation such one-dimensional model is introduced. The model originates from the recent theoretical advancements in the field of

Langevin dynamics driven by the spatially correlated noise (SCN). SCN can be linked to the diffusion in colloids or dynamic heterogeneity in molecular systems. Recently, it has been shown that the thermodynamic consistency requires SCN to be accompanied by the dissipation represented as the friction-response matrix. I will show that in the thermodynamic limit, this matrix can develop a genuine singularity in dissipation for finite volume packing, thus heralding the system jamming. Since this happens under the assumption of complete molecular disorder, this jamming is identified as the glass transition. The model introduces new perspective on the role of spatial correlations in vitrification, i.e. it shows that they might not be the consequence, but the cause of jamming. It also provides the exact relation between the noise correlation length and the critical packing. Finally, it suggests that the spectrum of the friction-response matrix might be the order parameter for the glass transition.

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The effects of sub-diffusion in the NTA size measurements of extracellular vesicles

Author: Maciej Majka[1]

[1] *Jagiellonian University*

Corresponding Author: maciej.majka@uj.edu.pl

The interest in the extracellular vesicles (EVs) is rapidly growing as they became reliable biomarkers for many diseases. For this reason, fast and accurate techniques of EVs size characterization are the matter of utmost importance. One increasingly popular technique is the Nanoparticle Tracking Analysis (NTA), in which the diameters of EVs are calculated from their diffusion constants. This assumes that the diffusion of EVs follows the Stokes-Einstein relation, i.e. that the Mean Square Displacement is linear in time (MSD$\propto t$). However, we show that this relation is severely violated in biological samples. In fact, at intermediate time periods MSD is strongly sub-diffusive (MSD $\propto t^{\alpha}$, $0 < \alpha < 1$). The sub-diffusive behaviour is well known in statistical physics, but most of its theoretical models do not provide the direct relation between the size of a particle and the generalized diffusion constant D_{α}. We solve this problem by introducing the logarithmic model of sub-diffusion. Applying it into analysis results in the average measured EV diameter reduced by 45% in comparison to the normal diffusion models. To corroborate our analysis, we compare our results with the AFM studies of the same samples. While the average size of EVs in AFM is still twice smaller than the in NTA, this discrepancy is expected due to the systematic differences between these two methods, which we also discuss.

Session 4 / **49**

Modelling heart rhytm variability in heart transplant patients by cellular automata on complex networks

Author: Danuta Makowiec[1]

[1] *Institute of Theoretical Physics and Astrophysics, University of Gdansk*

Corresponding Author: fizdm@univ.gda.pl

In patients with end-stage heart disease the heart transplantation (HTx) is associated with significant improvement in survival and in quality of life. However strong immunosuppressive drugs together with processes of aging could lead to vasculopathy and fibrosis of the donor heart. Moreover a spontaneous process of reinnervation proceeds in the myocardial tissue. All together impact on progressive alternations in the myocardial structure what influence propagation of activation wave fronts. A variety of arrhythmias – abnormal heart rhythm, may occur which adversely affect the patient long term survival.

Cellular automata modeling of signal propagation in the atrial muscle tissue is a rational compromise in resolving of physiological complexity, justified by efficiency in reproducing details of myocardial architecture. Consequently this modeling may explain key relationships between heart muscle structure and the propagation of activation wave fronts, possible reasons for the risk of arrhythmia.

Combining our proposition for stochastic network cellular automata model of the human pacemaker [1] and 2D cellular automata model of fibrosis in atria proposed in [2], we investigate which changes in myocardial structure affects propagation of cell-to-cell signals to contract in such way that we observe abnormal heart rhythm. 24-hour Holter measurement, a noninvasive and cheap ECG recording provides information on erratic rhythms of HTx patients. By modeling of structural alternates in the heart tissue we reproduce properties of some individual HTx patient heart rhythm [3].

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Session 12 / **36**

Dynamics of diluted confined systems

Author: Paolo Malgaretti[1]

[1] *Max Planck Institute for Intelligent Systems*

Corresponding Author: malgaretti@is.mpg.de

Recent studies have shown that the presence of boundaries can strongly affect the dynamics of physical systems.
For example, negative mobility and fluid recirculation occurs when an electrolyte is driven in a varying-section channels[1], rectification occurs active particles such as molecular motors[2] or active swimmers[3] moving in inhomogeneous environments and off–diagonal terms in the mobility tensor appears for binary mixtures of hard sphere confined between corrugated plates[4].
Clearly the interplay between the confined systems and the confining walls is maximized when the typical length scales of the confined system match with the size of the confining walls.
In this contribution I will discuss the general mechanisms at the basis of the interplay between the confined system and the confinement. In particular, by means of a few example I will show how analytical insight into the possible regimes can be attained.

Firstly, I will discuss how the electrostatic interaction between a tracer particle and the channel walls affect particle dynamics. In such a scenario, novel dynamical regimes such as negative mobility[1] and asymmetric passage times[5] can arise due to the interplay between the electrostatic interactions and the local entropic drive induced by the varying–section channel.

Secondly I will show how the insight gained by such studies can be transferred to the problem of polymer translocation across varying-section channels.
In particular, I will show that, under suitable approximation, it is possible to reduce the problem of polymer translocation across varying-section channels to that of a single point–like particle under

an effective potential that can be derived from the equilibrium local free energy of the polymer. Interestingly, the model predicts a non-monotonous dependence on the translocation time of the polymer across the pore appears. By comparing with Brownian dynamics simulations I will discuss the quantitative reliability of the point-like approximation as well as its regime of validity[6].

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Bayes' theorem and fluctuation theorems

Author: Michal Mandrysz[1]

[1] *Krakow*

Corresponding Author: michal.mandrysz@student.uj.edu.pl

Using Bayes' theorem we present a simple and general model which allows us to generate distributions of change in entropy between two macroscopic states. Obtained results are with agreement with the Second Law of thermodynamics, favouring decrease in the number of macroscopic states (keeping the number of microscopic states constant) and thus increasing the number of microscopic realisations of the surviving macrostates.
Due to the close resemblance of our expression to the fluctuation theorems we discuss its relation to Crooks Fluctuation Theorem. Surprisingly, the distributions obtained during experimental verification of Crooks relation on RNA strands follow closely the distributions obtained from our Bayesian relation.

Session 2 / 9

Temperature-abnormal diffusivity and weak ergodicity breaking in space-periodic systems driven by external forces

Author: Ivan Marchenko[1]

Co-authors: Andrey Zhiglo [2]; Igor Marchenko [3]; Victor Tkachenko [1]

[1] *National Scientific Centre "Kharkov Institute of Physics and Technology"*

[2] *The University of Tokyo*

[3] *NTU "Kharkov Polytechnic Institute"*

Corresponding Author: march@kipt.kharkov.ua

The phenomena of diffusion over a potential energy landscape play a key role in a number of processes in physics, chemistry and biology. In this talk a set of original theoretical results on diffusion enhancement of underdamped Brownian particles in symmetric space-periodic potential due to external forcing is presented [1-5].

We demonstrate that depending on the value of the constant external force in underdamped space-periodic systems dfferent functional dependences of the diffusivity on the temperature are realized. It is shown by numeric simulations of the Langevin equation that the phenomenon of diffusivity growth with the temperature decreasing ("temperature-abnormal diffusivity"- TAD) is manifested in a narrow interval of applied external forcing.
We demonstrate that weak ergodicity breaking takes place in TAD region. The correlation time tends to infinity as ~exp(+U/kBT) at T⟶0 in TAD region.
It is well-known that the double-well system is a typical classical memory device. We show that particle dynamics in underdamped space periodic systems may be considered as overdamped particle movement in effective double-well velocity space potential.
Based on the double-well model the analytical expression for diffusion coefficients in TAD region is derived. The functional dependence of TAD region width and its position on the friction coefficient and system parameters is found.
These results allow for simple experimental verification, and have practical applications – in physics of adsorbates, diffusion of interstitials, nanoparticle sorting, hydrogen energetics to name a few.

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Fast numerical method for Smoluchowski aggregation model with fragmentation terms

Author: Sergey Matveev[1]

Co-authors: Alexander Smirnov [2]; Artem Vladimirov [3]; Eugene Tyrtyshnikov [1]; Nadezda Vasilyeva [3]

[1] *Institute of Numerical Mathematics, RAS*

[2] *Lomonosov Moscow State University*

[3] *V.V. Dokuchaev Soil Science Institute*

Corresponding Author: matseralex@gmail.com

In this work we present an expansion of fast numerical method for Smoluchowski aggregation equations with additional unary fragmentation terms. The method is based on use of low-rank matrix decomposition of kernel kinetic coefficients and fast methods of linear algebra. We also present its application to local model of aggregation in soil profile and discuss results of our numerical experiments.

Session 7 / **137**

Stochastic dynamics in biological ion channels

Author: Peter McClintock[1]

Co-authors: Dmitri Luchinsky [1]; Igor Kaufman [1]; Olena Fedorenko [2]; Robert Eisenberg [3]; Stephen Roberts [2]; William Gibby [1]

[1] *Department of Physics, Lancaster University*

[2] *Department of Biomedical and Life Sciences, Lancaster University*

[3] *Department of Molecular Biophysics, Rush University, Chicago*

Corresponding Author: p.v.e.mcclintock@lancaster.ac.uk

The passage of ions through biological cell membranes [1] is essential for life at all levels. It occurs via ion channels through proteins embedded in the membrane, and involves Brownian motion under the influence of powerful electrostatic forces. The permeation process is highly selective, e.g. in valence selectivity a calcium channel selects Ca^{2+} over Na^{+} by up to 1000:1. There is still no general agreement on the physical mechanism(s) underlying selectivity, but it is known to be associated with fixed negative charge Q_f in a narrow part of the channel called the selectivity filter. There are persuasive arguments [2] that valence selectivity arises from ionic Coulomb blockade (ICB), a phenomenon that is closely analogous to electronic Coulomb blockade in semiconductor devices such as quantum dots and which gives rise to distinct conduction bands and stop-bands as Q_f is varied. We report the first systematic tests [3] of the ICB picture based on experimental, analytical and numerical investigations of the influences of the fixed charge and bulk ionic concentrations on conduction and selectivity in the bacterial NaChBac channel and its mutants. Site-directed mutagenesis and voltage clamp recordings were used to investigate its Na^{+}/Ca^{2+} selectivity, divalent blockade and anomalous mole fraction effect (AMFE). We show that an enhanced ICB model can describe well both the main experimental observations (divalent blockade and AMFE) and the results of Brownian dynamics simulations including the conduction bands and concentration-dependent shifts of the Coulomb staircase of channel occupation. We take account of multi-ion effects, the discreteness of the ionic energy levels, their occupation statistics, and the density of states in the channel, and we consider a generalisation of the theory to encompass selectivity between alike charges [4,5]. These results are not only extending the understanding of ion channel selectivity but also promise applications to biomimetic nanopores with charged walls.

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Session 4 / **76**

Large deviations of surface height in the Kardar-Parisi-Zhang equation

Author: Baruch Meerson[1]

[1] *Hebrew University of Jerusalem*

Corresponding Author: meerson@mail.huji.ac.il

The Kardar-Parisi-Zhang (KPZ) equation describes an important universality class of nonequilibrium stochastic growth. There has been much recent interest in the one-point probability distribution P(H,t) of height H of the evolving interface at time t. I will show how one can use the optimal fluctuation method (also known as the instanton method, the weak-noise theory, the macroscopic fluctuation theory, or simply WKB) to evaluate P(H,t) for different initial conditions in 1+1 dimensions. At short times the body of the height distribution is Gaussian, but its tails are non-Gaussian and highly asymmetric. In a moving frame, one of the tails coincides, at all times, with the proper tail of the Tracy-Widom distribution (for the flat and curved interface), and of the Baik-Rains distribution (for the stationary interface). The other tail displays a behavior that differs from the known long-time asymptotic. At sufficiently large |H| this large-deviation tail also persists at arbitrary long times. The case of stationary interface is especially interesting. Here at short times the large deviation function of the height exhibits a singularity at a critical value of |H|. This singularity results from a symmetry-breaking of the "optimal path" of the system, and it has the character of a second-order phase transition.

Session 4 / **47**

Anomalous diffusion, ageing, and non-errodicity

Author: Ralf Metzler[1]

[1] *University of Potsdam*

Corresponding Author: rmetzler@uni-potsdam.de

In 1905 Einstein formulated the laws of diffusion, and in 1908
Perrin published his Nobel-prize winning studies determining Avogadro's number from diffusion measurements. With similar, more refined techniques the diffusion behaviour in complex systems such as the motion of tracer particles in living biological cells is nowadays measured with high precision. Often the diffusion turns out to deviate from Einstein's laws. This talk will discuss the basic mechanisms leading to anomalous diffusion as well as point out the physical consequences. In particular the unconventional behaviour of non-ergodic, ageing systems will be discussed within the framework of different stochastic processes. Concrete examples include granular gases, biological cells, lipid membranes, and interacting many particle systems.

Session 12 / **75**

Mean-potential law in evolutionary games

Authors: Jacek Miekisz[1]; Paweł Nałęcz-Jawecki[2]

[1] *Institute of Mathematics, Polish Academy of Sciences and University of Warsaw*

[2] *University of Warsaw*

Corresponding Author: miekisz@mimuw.edu.pl

We formulate two simple and intuitive criteria for evolutionary stability of pure Nash equilibria in stochastic dynamics of finite populations. Our approach is based on the mapping of continuous stochastic dynamics into discrete ones and the appropriate choice of potential functions. We present the correspondence between one-dimensional stochastic differential equations describing diffussion with a state-dependent drift and discrete-space random walks, which is exact even in finite-state spaces. This enables us to compute fixation probabilities in various stochastic dynamical systems with two absorbing states.

Session 9 / **72**

Diffusion and dynamic scaling in concentrated charge-stabilized colloidal suspensions

Author: Gerhard Naegele[1]

Co-authors: Adolfo J. Banchio [2]; Marco Heinen [3]; Mariano Brito [1]

[1] *Forschungszentrum Jülich, ICS-3*

[2] *FaMAF-UNC and IFEG-CONICET, University of Cordoba, Argentina*

[3] *University of Guanajuato at Leon, Mexico*

Corresponding Author: g.naegele@fz-juelich.de

We present a joint theory, simulation and experimental study of collective and self-diffusion in concentrated suspensions of charged colloidal particles. The study is based on the generalized Smoluchowski diffusion equation accounting both for direct and solvent-mediated hydrodynamic interactions, and it spans the range from the colloidal short-time to the long-time regime. Owing to the large size asymmetry between the colloidal macroions and the neutralising microns, the degrees of freedom of the latter can be integrated out, resulting in an effective (microion-dressed) colloid pair potential characterised by a renormalised colloid charge and Debye screening parameter. Various state-of-the-art methods of calculating such an effective colloid interaction potential are compared for suspensions in osmotic equilibrium with a salt reservoir. The effective colloid potential is used as input in our accelerated Stokesian Dynamics (ASD), Brownian Dynamics (BD) and self-consistent mode-couling theory (MCT) calculations of intermediate and self-intermediate scattering functions and particle mean-squared displacements. On basis of these numerical results that are compared in addition with dynamic light scattering data on silica particles suspensions, the influence of hydrodynamic interactions on self- and collective diffusion, and the accuracy of the MCT method are quantified. A proposed time-wavenumber scaling relation between short- and long time diffusion properties is shown to be violated in general.

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Reinventing the triangle: rule of thumb for assessing detectability of communities in networks

Author: Jeremi Ochab[1]

[1] *M. Smoluchowski Institute of Physics, Jagiellonian University, Kraków*

Corresponding Author: jeremi.ochab@uj.edu.pl

Statistical significance of network clustering has been an unresolved problem since it was observed that community detection algorithms produce false positives even in random graphs. After a phase transition between undetectable and detectable cluster structures was discovered [1,2], the spectra of adjacency matrices and detectability limits were shown to be connected, and they were calculated for a wide range of networks with community structure [3]. In practice, given a real-world network neither the hypothetical network model nor its full eigenspectrum is known, and whether the network has any detectable communities cannot be easily established.

Based on the global clustering coefficient (GCC) we construct a criterion telling whether in an undirected, unweighted network there is some/no detectable community structure, or if the network is in a transient regime. To that end we use approximations of GCC and the spectra of adjacency matrices, together with the empirical observations showing that: a) for graphs with community structure GCC reaches the random graph value before its connectivity is fully random, and b) this saturation of GCC coincides with the theoretically predicted limit of detectability.

We compare the criterion against existing methods of assessing significance of network partitioning. We compute it on various benchmark graphs, as well as on real-world networks from SNAP database,

and compare it with the results of state-of-the-art community detection methods. The method is simple and faster than methods involving bootstrapping; it is robust also on sparse networks. Analogous criteria are plausible also for directed graphs.

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Session 5 / **96**

Stochastic gene expression in cells undergoing division

Author: Jakub Jędrak[1]

Co-author: Anna Ochab-Marcinek [1]

[1] *Institute of Physical Chemistry, Polish Academy of Sciences*

Corresponding Author: ochab@ichf.edu.pl

Stochasticity in gene expression is one of the most important problems of quantitative biology. It has been shown that, in the systems as small as living cells, production of proteins is strongly affected by random fluctuations coming from various sources. As a result, the biological noise is a meaningful factor influencing cellular processes and cell-fate decisions. The particular questions explored within the field of quantitative biology are, among others, the correct identification of noise sources and correct estimation of noise parameters, e.g., frequencies and sizes of the random bursts of protein production.

We propose a stochastic model of gene expression in cells undergoing division. The model combines a deterministic approximation of protein degradation and the two sources of noise: 1) Random bursts of protein production, and 2) more or less random duration of the cell cycle. Random partitioning of proteins between daughter cells is also possible as the third source of noise.

In the classical model proposed by the Xie group, the effect of cell division was tacitly identified with the effect protein degradation. We show that this may not be a correct assumption and the values of mean burst size and mean burst frequency inferred from the experiments using the classical model may be wrong. We show that our model provides more reasonable estimates for these quantities. Moreover, our model demonstrates that the "noise floor", observed in the experiments and previously ascribed to an unidentified extrinsic noise, may be the effect of cell division. Our model sets physical constraints, based on the degree of randomness in cell cycle duration, for the levels of noise in gene expression.

Session 6 / **24**

Griffiths phases on a large human Open Connectome network

Author: Geza Odor[1]

Co-author: Michael Gastner [2]

[1] *MTA-EK-MFA, Research Center for Energy, Hungarian Academy of Sciences*

[2] *Yale-NUS College, 16 College Avenue West, 01-220 Singapore 138527*

Corresponding Author: odor@mfa.kfki.hu

Extended numerical simulations of threshold models have been performed on a human brain network with
N=836733 connected nodes available from the Open Connectome Project [1]. While in the case of simple
spreading models like contact process, SIS or threshold model a sharp discontinuous phase transition, without any critical dynamics arises, variable threshold models exhibit extended power-law scaling regions. This is attributed to fact that Griffiths effects, stemming from the topological or interaction heterogeneity of the network, can become relevant if the input sensitivity of nodes is equalized. Nonuniversal power-law avalanche size and time distributions have been found with exponents agreeing with the values obtained in electrode experiments of the human brain [2]. Power-law activity time dependences occur sub-critically in an extended control parameter space region without the assumption of self-organization. Probably the most important result of this study is that negative weights enable local sustained activity and promote strong rare-region effects without network fragmentation. Thus, connectomes with high graph dimensions can be subject to rare-region effects and can show measurable Griffiths effects. Another important observation is that power-laws may occur in a single network, without sample averaging, due to the modular topological structure. Link directness, as well as the consequence of inhibitory connections is studied. Robustness with respect of random removal of links suggest that connectome generation errors do not modify the Griffths effects qualitatively.

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Session 5 / **21**

Order in quantum compass and orbital e_g models

Author: Andrzej M. Oles[1]

Co-authors: Jacek Dziarmaga [1]; Piotr Czarnik [1]

[1] *Jagiellonian University*

Corresponding Author: a.m.oles@uj.edu.pl

Exchange interactions in orbital models are frustrated even on a
square lattice, where two $T = 1/2$ pseudospin components
$T_i^\gamma(\theta)$ parameterized by angle $\theta \in (0, \pi/2]$ interact by terms $JT_i^\gamma(\theta)T_j^\gamma(\theta)$.
Maximal frustration in the quantum compass model with
$T_i^\gamma(\pi/2) \equiv \frac{1}{2}\sigma_i^\gamma$, where
σ_i^γ is the Pauli matrix, is reduced to moderate
frustration for the e_g orbital model at $\theta = \pi/3$ [1].
We investigate thermodynamic phase transitions at temperature T_c
on an infinite square lattice by variational tensor network renormalization (VTNR) in imaginary time. From the linear susceptibility (order parameter) in the symmetric (symmetry-broken) phase the onset of nematic order in the quantum compass model is estimated at $T_c/J = 0.0606(4)$ [2], in good agreement with Quantum Monte Carlo (QMC). For the 2D e_g orbital model one finds: (i) a very accurate VTNR estimate of $T_c/J = 0.3566 \pm 0.0001$ while QMC fails due to the sign problem, and (ii) that the critical exponents are within the Ising universality class. Remarkably large difference in frustration and entanglement results in so distinct T_c.

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Critical behavior of noise-induced phase synchronization

Author: Pedro Pinto[1]

Co-authors: Andre Penna [2]; Fernando Oliveira [2]

[1] *Universidade Federal do Oeste da Bahia*

[2] *Universidade de Brasília*

Corresponding Author: faooliveira@gmail.com

We present for the first time in detail the set of the main critical exponents associated with the phase transition of the Kuramoto model under multiplicative noise action. This was done considering the equilibrium thermodynamics for the states of synchronization [1], as well as the subsequent analysis of the critical behavior of the free energy and entropy of the model. We reinforce the concept of the synchronization field for a system of oscillators with multiplicative noise where an expression for the susceptibility is analytically obtained at the critical limit. These results complete the gap that was lacking in obtaining all the critical exponents associated with the phase transition of a Kuramoto-type model.

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Pendular behaviour of public transport network

Author: Mirian Izawa[1]

Co-authors: Bernardo Mello [1]; Daniel Cajueiro [1]; Fernando Oliveira [1]

[1] *Universidade de Brasília*

Corresponding Author: faooliveira@gmail.com

In this work, we propose a methodology that bears close resemblance to the Fourier analysis of the first harmonic to study networks subjected to pendular behavior [1]. In this context, pendular behavior is characterized by the phenomenon of people's dislocation from their homes to work in the morning and people's dislocation in the opposite direction in the afternoon. Pendular behavior is a relevant phenomenon that takes place in public transport networks because it may reduce the overall efficiency of the system as a result of the asymmetric utilization of the system in different directions. We apply this methodology to the bus transport system of Bras\'{i}lia (Brazil), which is a city that has commercial and residential activities in distinct boroughs. We show that this methodology can be used to characterize the pendular behavior of this system, identifying the most critical nodes and times of the day when this system is in more severe demanded[1,2].

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Session 9 / 87

Exact solution for a $1+1$ etching model.

Author: Fernando Oliveira[1]

Co-authors: Evandro Rodrigues [1]; Ismael Costa [1]; Waldenor Gomes [1]; Washington Alves [1]

[1] *Universidade de Brasília*

Corresponding Author: faooliveira@gmail.com

We present a method to derive analytically the growths exponents of a eroded surface whose dynamics is ruled by cellular automata. Starting from the automata, we write down the time evolution for the height's average and height's variance (roughness). We apply the method to the etching model[1,2] of $1+1$ dimensions, than we obtain the dynamical exponents, which perfectly match the numerical results obtained from simulations. Those exponents are exact and they are the same as those exhibited by the KPZ model[3] for this dimension. Therefore, it shows that the etching model and KPZ belong to the same universality class[4]. Moreover, we proof that in the continuous limit the majors terms leads to KPZ [5].

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Session 8 / **111**

Diffusive escape through a narrow opening: new insights into a classic problem

Author: Gleb Oshanin[1]

Co-author: Denis Grebenkov [2]

[1] *Laboratoire de Physique Théorique de la Matière Condensée (UMR CNRS 7600) Sorbonne Universités - UPMC, Paris, France*

[2] *Laboratoire de Physique de la Matiere Condensee Ecole Polytechnique, F-91128 Palaiseau France*

Corresponding Author: oshanin@lptmc.jussieu.fr

In this talk I overview our recent results [1] on the mean first escape time T of a diffusive particle from a spherical (or a circular) domain enclosed by an impenetrable boundary containing a small escape window. Our settings differ from the classical narrow escape problem in two aspects : First, we introduce explicitly into the model long-range potential interactions of a particle with the boundary, which are always present in realistic situations. Second, we take into account effects of an energy/entropy barrier at the escape window, which were discarded in previous analyses. We develop a self-consistent approximation to derive for T a general expression, akin to the celebrated Collins-Kimball relation in chemical kinetics, which shows that the contibution due to a diffusive search for the escape window and the contribution due to the passage through the escape window are additive. Further on, our analysis reveals that in the true narrow escape limit, where the size of the opening tends to zero, the barrier-induced contribution to T represents the dominant controlling factor such that the narrow escape problem is « barrier-limited » rather than « search-limited ». Next, we analyse the contribution due to diffusive search for the escape window and construct

an expansion in powers of the size of the escape window in which the coefficients before the leading terms are expressed as integrals and derivatives of (a rather arbitrary) interaction potential. On example of a triangular-well potential we show that the contribution to T due to diffusive search is non-monotonic with respect to the range of the interaction potential, being minimal for the one having an intermediate extent, neither too concentrated on the boundary nor penetrating too deeply into the bulk. Our analytical predictions are confirmed by numerical simulations.

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Session 12 / **104**

Stochastic processes for fractional kinetics with application to anomalous diffusion in living cells

Author: Gianni Pagnini[1]

Co-authors: Carlo Manzo [2]; Daniel Molina-García [1]; Paolo Paradisi [3]

[1] *BCAM - Basque Center for Applied Mathematics, Bilbao, Basque Country - Spain*

[2] *Universitat de Vic - Universitat Central de Catalunya (UVic-UCC), Vic, Spain*

[3] *ISTI - CNR, Pisa, Italy*

Corresponding Author: gpagnini@bcamath.org

Fractional kinetics is derived from Gaussian processes when the medium where the diffusion takes place is characterized by a population of length-scales [1]. This approach is analogous to the generalized grey Brownian motion [2], and it can be used for modelling anomalous diffusion in complex media. In particular, the resulting stochastic process can show sub-diffusion, ergodicity breaking, p variation, and aging with a behaviour in qualitative agreement with single-particle tracking experiments in living cells. Moreover, for a proper distribution of the length-scales, a single parameter controls the ergodic-to-nonergodic transition and, remarkably, also drives the transition of the diffusion equation of the process from nonfractional to fractional, thus demonstrating that fractional kinetics emerges from ergodicity breaking [3].

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Session 5 / **128**

Nonequilibrium steady states in Langevin thermal systems

Author: Hyunggyu Park[1]

Co-author: Hyunn Keun Lee [2]

[1] *Korea Institute for Advanced Study*

[2] *SungkyunKwan University*

Corresponding Author: hgpark@kias.re.kr

Equilibrium is characterized by its fundamental properties such as the detailed balance, the fluctuation-dissipation relation, and no heat dissipation. Based on the stochastic thermodynamics, we show that these three properties are equivalent to each other in conventional Langevin thermal systems with microscopic reversibility. Thus, a conventional steady state has either all three properties (equilibrium) or none of them (nonequilibrium). In contrast, with velocity-dependent forces breaking the microscopic reversibility, we prove that the detailed balance and the fluctuationdissipation
relation mutually exclude each other and no equivalence relation is possible between any
two of the three properties. This implies that a steady state of Langevin systems with velocitydependent
forces may maintain some equilibrium properties but not all of them. Our results are
illustrated with a few example systems.

Session 12 / **118**

Bottlebrush polymers: from dilute solutions to super-soft rubbers

Author: Jaroslaw Paturej[1]

Co-authors: Joanna Burdyńska [2]; Krzysztof Matyjaszewski [2]; Michael Rubinstein [3]; Panyukov Sergey [4]; Sergei Sheiko [3]; Torsten Kreer [5]; William Daniel [3]

[1] *University of Szczecin*

[2] *Carnegie Mellon*

[3] *University of North Carolina*

[4] *Russian Academy of Sciences*

[5] *Leibniz Institute of Polymer Research Dresden*

Corresponding Author: jpaturej@univ.szczecin.pl

Polymer bottlebrushes provide intriguing features being relevant both in nature and in synthetic systems. While their presence in the articular cartilage optimizes synovial joint lubrication, bottlebrushes offer pathways for fascinating applications, such as within super-soft elastomers or for drug delivery. However, the current theoretical understanding lacks completeness, primarily due to the complicated interplay of many length scales. During the talk new analytical model of bottlebrush polymers will be presented. The model applies to solutions ranging from dilute concentrations to dense melts. The validity of our model is supported by data from extensive molecular dynamics simulation. We demonstrate that the hierarchical structure of bottlebrushes dictates a sequence of conformational changes as the solution concentration increases. The effect is mediated by screening of excluded volume interactions at subsequent structural parts of the bottlebrushes. Our findings provide important insights that should enable improved customization of novel materials based on the architectural design of polymer bottlebrushes.

Session 3 / **191**

Aerated Poisson distributions and their exact approximants.

Author: Karol Penson[1]

[1] *University Paris 6*

Corresponding Author: penson@lptl.jussieu.fr

We analyze the properties of combinatorial numbers appearing in the normal ordering of powers of certain differential operators. They are natural generalizations of the conventional Bell numbers. We explicitly construct the solutions of the Stieltjes moment problems with these combinatorial sequences. It turns out that in certain cases one encounters as solutions the discrete probability distributions based on lacunary subsets of positive integers. They generalize the standard Poisson laws and are called aerated Poisson distributions. We furnish explicit approximants of the aerated Poisson distributions through continuous functions via reparametrization of auxiliary solutions for other generalized Bell numbers.

EPS / **175**

What is Complexity?

Author: Grassberger Peter[1]

[1] *Forschungszentrum Juelich*

Corresponding Author: p.grassberger@fz-juelich.de

We have now institutes for complex systems, conferences on complex systems, and journals of complex systems. So most of us have a good feeling what is a complex system. But what is complexity itself, and is there any way to measure it? The answer to this is surprisingly non-trivial. Indeed, there is no universally agreed concept, according to which a bacterium is more complex than a human. But how can we do complex systems science, if we cannot measure complexity? How would we do thermodynamics, if we could not measure temperature? In this talk I will not give answers, but I will discuss several approaches that give partial answers at least.

Session 3 / **81**

Fluctuating hydrodynamics of one-dimensional nonlinear chains

Author: Harald Posch[1]

Co-author: Henk van Beijeren [2]

[1] *University of Vienna*

[2] *Utrecht University*

Corresponding Author: harald.posch@univie.ac.at

One-dimensional particle systems are known to be anomalous with respect to the dynamics of their hydrodynamic conserved fields and their related currents. We review some of the predictions of mode-mode coupling theory combined with exact results by Prähofer and Spohn [J. Stat. Phys., vol. 115, 255 (2004)] to derive asymptotic expressions for the time-correlation functions of the hydrodynamic modes and their currents. These results are compared to extensive computer simulations for two simple fluids with non-linear short-range interactions.

Session 7 / **86**

Identification of spatial diffusivity patches by the wavelet processing of single-particle trajectories

Author: Eugene Postnikov[1]

Co-author: Igor Sokolov [2]

[1] *Kursk State University*

[2] *Humbold University at Berlin*

Corresponding Author: postnicov@gmail.com

Modern developments in single particle tracking not only open new perspectives for the study of molecular motions in complex environments,
but also allow for using these motions as a probe for revealing properties of substrates on which the motions occur. This approach is
especially important for studying biological membranes since their non-uniform structure (e.g. due to the presence of protein clusters)
results in a large variety of anomalous diffusion phenomena [1]. The first step on this way is providing a map of local
diffusion coefficients. Using a standard approach based on moving time averaging of the local squared displacements poses a task of
judicious choice of the averaging window, which, for achieving satisfactory accuracy, has to be chosen adaptively, depending on the local diffusion coefficient itself.

This complication may be circumvented by generalizing methods of robust linear fitting based on comlexification of the smooth functions
with their subsequent Fourier [2] or Complex Wavelet Transforms (CWT) [3]. For this aim the function $\exp[i\Omega R^2(t)]$,
where $R^2(t)$ is the step-wise displacement squared and Ω is an appropriately chosen factor, is used as an input for the CWT.
A modification with respect to [3] is the replacement of the Morlet wavelet
by a combination of the Tukey window and the multiplicative decomposition of the exponential factor that assures better spatio-temporal localization.

The method proposed was checked in numerical simulations of random walks on patchy structures with different diffusion coefficients within patches,
and was shown to be able to reveal patched structure of diffusion coefficient and to distinguish such situations from random walks with a
time-dependent diffusion coefficient. In addition, the method was applied to the experimental data of [1] provided by courtesy of C. Manzo.
Its application resulted not only in the demonstration of an existence of substrate patches with slowly varying diffusivity but also allowed for a discussion
of a difference between such structures and systems with ergodicity breaking.

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EPS / **167**

A bird's eye view of Nonlinear Physics

Author: Itamar Procaccia[1]

[1] *The Weizmann Institute of Science*

Corresponding Author: itamar.procaccia@gmail.com

The special challenge of Nonlinear Physics is that every new problem calls for a specialized idea and a new method to solve it. There exist almost no "general" methods in the arsenal. I will review my own forays into the nonlinear domain stressing this challenge and highlighting the few lucky strikes that I had been involved in during more than 35 years of research.

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The q-voter model with nonconformity in freely forming groups: does the size distribution matters?

Author: Wojciech Radosz[1]

Co-authors: Adam Mielnik-Pyszczorski [2]; Katarzyna Weron [2]; Marta Brzezińska [2]

[1] *Wrocław University of Science and Technology*

[2] *Wroclaw University of Science and Technology*

Corresponding Author: wojciech.radosz@pwr.edu.pl

We study a q-voter model with stochastic driving on a complete graph with q being a random variable described by probability density function P(q), instead of a constant value. We investigate two types of P(q): (1) artificial with the fixed expected value < q >, but a changing variance and (2) empirical of freely forming groups in informal places. We investigate also two types of stochasticity that can be interpreted as different kinds of nonconformity (anticonformity or independence) to answer the question about differences observed at the macroscopic level between these two types of nonconformity in real social systems. Moreover, we ask the question if the behavior of a system depends on the average value of the group size q or rather on probability distribution function P(q).

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Complex dynamics of guest molecules in all-optical poling: kinetic Monte Carlo modelling

Author: Wojciech Radosz[1]

Co-authors: Antoni C. Mituś [2]; Grzegorz Pawlik [3]

[1] *Wrocław University of Science and Technology*

[2] *Wroclaw University of Science and Technology*

[3] *Wroclaw University of Science and Technology,*

Corresponding Author: wojciech.radosz@pwr.edu.pl

We study theoretically the kinetics of non-interacting photo-switchable guest molecules (model azo-dye) dispersed in host (model polymer matrix) in the all-optical poling process close to the glass transition temperature Tg. The polymer matrix is simulated using the bond-fluctuation model. The kinetics of multiple trans-cis-trans cycles is formulated in terms of transition probabilities which depend on local free volume in the matrix and its dynamics. Close to Tg complex dynamics of guest molecules is observed, what implies the presence of dynamic heterogeneities of the matrix in space

and time which influences guest molecules. A qualitative physical picture of mosaic-like states - intertwined areas of free- and hindered angular motion of guest molecules - is proposed and the role of related short and longer scales in space for the promotion of complex dynamics of guest molecules is discussed.

Session 12 / **32**

Forces from temperature quenches in thermal and active matter

Author: Christian Rohwer[1]

Co-authors: Alexandre Solon [2]; Matthias Krüger [1]; Mehran Kardar [2]

[1] *Max Planck Institute for Intelligent Systems*

[2] *MIT*

Corresponding Author: crohwer@is.mpg.de

Non-equilibrium systems are known to exhibit long-ranged correlations in the presence of dynamical conservation laws. This phenomenon gives rise to various types of fluctuation-induced forces between objects immersed in non-equilibrium media. However, driving systems out of equilibrium, for instance by changing their temperature, may also result in changes of the mean density.

In this talk I will discuss our recent work on non-equilibrium fluctuation-induced (Casimir) forces [1,2] and density-induced forces [2] arising from temperature quenches in thermal and active matter. Focusing on temperature quenches, we predict theoretically and demonstrate with simulations the existence of both these types of forces between objects immersed in a conserved density. (In active matter, a quench could be achieved by a rapid change in activity.) We discuss the distinguishing features of fluctuation-induced and density-induced forces as regards universality, time-scales and scaling. By considering microscopic theories and coarse-graining procedures, we propose methods to extract the fluctuation-induced contribution of forces in simulations. Simulation results [2] display the scaling in space and time predicted in [1].

[1] C.M. Rohwer, M. Kardar, M. Krüger, Phys. Rev. Lett. 015702 **118** (2017)

[2] C.M. Rohwer, A. Solon, M. Kardar, M. Krüger, *in preparation* (2017)

EPS / **146**

Generic properties of stochastic entropy production

Author: Edgar Roldan[1]

Co-authors: Frank Jülicher [1]; Izaak Neri [1]; Simone Pigolotti [2]

[1] *Max Planck Institute for the Physics of Complex Systems*

[2] *Okinawa Institute for Science and Technology*

Corresponding Author: edgar@pks.mpg.de

The laws of thermodynamics can be extended to mesoscopic systems for which energy changes are on the order of the thermal energy are relevant. Therefore, thermodynamic observables associated with mesoscopic degrees of freedom are stochastic. A key example of such thermodynamic

observable is the stochastic entropy production in nonequilibrium processes. Little is known beyond fluctuation theorems about universal or model-independent statistics of entropy-production fluctuations.

Using Martingale theory we have discovered novel universal statistics of stochastic entropy production in nonequilibrium steady states such as: (i) The distribution of the negative record (which we call infimum) of entropy production (ii) the passage probabilities of entropy production; (iii) the stopping-time fluctuations of entropy production.

For nonequilibrium Langevin processes, we derive an Ito stochastic differential equation for entropy production. Introducing a random-time transformation, entropy production obeys a one-dimensional drift-diffusion equation, independent of the underlying physical model. This transformation allows to identify novel generic properties of entropy production. It also leads to an exact uncertainty equality relating the Fano factor of entropy production and the Fano factor of the random time.

Our results have interesting implications for stochastic processes that can be discussed in colloidal systems and active molecular processes. For example, we make predictions for the distribution of the maximum backtrack depth of RNA polymerases during RNA transcription in eukaryotes.

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Session 1 / **60**

Entropy facilitated active transport

Author: J. Miguel Rubi[1]

[1] *University of Barcelona*

Corresponding Author: mrubi@ub.edu

We show how active transport of ions can be interpreted as an entropy facilitated process. In this interpretation, a particular change in the pore geometry through which substrates are transported gives rise to a driving force. This chemical energy provided by the chemical reaction is then used to create a protein geometry favorable for the uphill transport of ions. Attempts to estimate the energy available by this change in several proteins shows that an entropic contribution from the pore geometry is significant. We discuss how this effect can be used to understand how energy transduction in active transport can take place over a relatively long distance.

Session 8 / **44**

Out-of-equilibrium physics in spontaneous synchronization

Author: Stefano Ruffo[1]

Co-authors: Alessandro Campa [2]; Shamik Gupta [3]

[1] *SISSA*

[2] *Istituto Superiore di Sanità, Roma*

[3] *Department of Physics, Ramakrishna Mission Vivekananda University, Kollkata, India*

Corresponding Author: ruffo@sissa.it

Spontaneous synchronization is a cooperative phenomenon common in nature which makes oscillators of different frequencies, if strongly coupled, operate together with a single common frequency. Such cooperative effects occur in physical and biological systems over length and time scales of several orders of magnitude. Examples: are flashing of fireflies, rhythmic applause in a concert hall, animal flocking behavior, electrical power-grids, etc. The most celebrated model of synchronization is the Kuramoto model, introduced in 1975, which is simple enough to allow quite a detailed analytical treatment, at the same time capturing several features of realistic systems. After discussing the general dynamical and statistical features of synchronization, I will concentrate on its out-of-equilibrium physical aspects when uncorrelated Langevin noise is added to the model.

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Theory of microwave amplifier based on single Josephson junction

Author: Artem Ryabov[1]

Co-authors: Martin Žonda [1]; Tomáš Novotný [1]

[1] *Charles University, Faculty of Mathematics and Physics, Department of Condensed Matter Physics, Prague, Czech Republic*

Corresponding Author: rjabov.a@gmail.com

We present a theory describing the recently proposed and realized microwave amplifier based on the negative resistance of a damped Josephson junction [P. Lahteenmaki et al., Sci. Rep. 2, 276 (2012)]. The standard linear response theory based on expansion around the limit cycle [A. Kamal et al. Phys. Rev. B 86, 144510 (2012)] yields nearly perfect results for the gain characteristics of the device, but it fails to describe a reported noise suppression at the working frequency of the amplifier. In order to capture the latter effect, we extend the linear response theory to account for a subtle interplay between linear fluctuations around the limit cycle and nonlinear dynamics of the phase along the limit cycle. Detailed comparison of our predictions with the experiment and implications of these findings on the prospects of achieving the originally intended quantum-limited amplification will be discussed.

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Power and efficiency of Feynman ratchet

Author: Ekaterina Berestneva[1]

Co-authors: Artem Ryabov [1]; Viktor Holubec [1]

[1] *Charles University*

Corresponding Authors: rjabov.a@gmail.com, despvir@gmail.com

We focus on an overdamped two-dimensional diffusion of a particle in a corrugated tilted periodic potential. The particle is subjected to two white noise sources with different intensities representing two heat baths at different temperatures. The model dynamics mimics a working principle of the famous Feynman ratchet and pawl. Using a perturbation expansion in potential width, which is

similar in spirit to Fick-Jacobs theory, we obtain stationary probability current, mean velocity of the particle and also discuss energetics of the ratchets including its output power and efficiency.

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[2] A. Ryabov, V. Holubec, M. H. Yaghoubi, M. Varga, M. E. Foulaadvand and P. Chvosta, Transport coefficients for a confined Brownian ratchet operating between two heat reservoirs, J. Stat. Mech. 2016, 093202, 2016

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Non-monotonic temperature dependence of diffusion coefficient in tilted disordered potentials

Author: Raul Salgado-Garcia[1]

[1] *Universidad Autonoma del Estado de Morelos*

Corresponding Author: raulsg@uaem.mx

We study the transport properties of non-interacting overdamped particles, moving on tilted disordered potentials, subjected to Gaussian white noise. We give exact formulas for the drift and diffusion coefficients for the case of random potentials resulting from the interaction of a particle with a "random polymer". In our model the random polymer is made up, by means of some stochastic process, of monomers that can be taken from a finite or countable infinite set of possible monomer types. For the case of uncorrelated random polymers we found that the diffusion coefficient exhibits a non- monotonous behavior as a function of the noise intensity. Particularly interesting is the fact that the relative diffusivity becomes optimal at a finite temperature, a behavior which is reminiscent of stochastic resonance. We explain this effect as an interplay between the deterministic and noisy dynamics of the system. We test our findings by means of numerical simulations of the corresponding Langevin dynamics of an ensemble of noninteracting overdamped particles diffusing on uncorrelated random potentials

EPL / 53

Random matrices meet trapped fermions

Author: Gregory Schehr[1]

[1] *Universite Paris-Sud, CNRS*

Corresponding Author: gregory.schehr@u-psud.fr

I will review some recent results exploring the connection between non-interacting fermions in a d-dimensional trapping potential and random matrix theory. The presence of the trap introduces an edge where the average density of fermions vanishes. Far from the edge, near the centre of the trap (the so called "bulk regime"), physical properties of the fermions have traditionally been understood using the Local Density Approximation. However, this approximation drastically fails near the edge where the density vanishes. In this talk, I will show that, even near the edge, novel universal properties emerge, independently of the details of the confining potential. These universal correlations can be described by random matrix theory (in one dimension and at zero temperature) and by more general determinantal processes in higher dimensions and finite temperature.

D. S. Dean, P. Le Doussal, S. N. Majumdar, G. Schehr, Phys. Rev. Lett. **114**, 110402 (2015),
EPL **112**, 60001 (2015),
Phys. Rev. A **94**, 063622 (2016).

Session 9 / **138**

Eliminating inertia of a stochastic microswimmer with constant speed

Author: Lutz Schimansky-Geier[1]

Co-authors: Igor M. Sokolov [1]; Jörg Nötel [1]

[1] *Department of Physics, Humboldt-University at Berlin*

Corresponding Author: alsg@physik.hu-berlin.de

An often used model for an active entity is the two dimensional stochastic microswimmer. It moves due to a propulsive mechanism with constant speed and changes the direction due to deterministic and random torques. Despite the simplicity, the model it is not an overdamped situation. Intertia is reflected by an initial ballistic behaviour. Only after an crossover time being the relaxation time of the orientational directions the motion becomes normally diffusive characterized by a diffusion coefficient.

In the report I discuss the properties and the distribution of displacements of the stochastic microswimmer with constant speed. Various situations with several random torques like Gaussian white noise, an Ornstein-Uhlenbeck process and alpha-stable noise will be studied. Special attention is devoted to the adiabatic elimination of inertia in the model and the derivation of the overdamped limit. It results for all types of random torques in a Gaussian simplification similar to a Brownian particle driven by white noise. Therein the noise intensity addresses the specific noise sources.

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S. Milster, J. Nötel, I.M. Sokolov, L. Schimansky-Geier, „Eliminating inertia in a stochastic model of a microswimmer with constant speed“, Eur. Phys. J. Special Topics **226**, 2039-2055 (2017).

J. Nötel, I.M. Sokolov, L. Schimansky-Geier, „Gaussian appproximation of the stochastic microswimmer driven by alpha-stale noise, submitted for publication.

Session 5 / **176**

Transport of granular materials in turbulent flows (or sand in streams)

Author: Rina Schumer[1]

[1] *Desert Research Institute*

Corresponding Author: rina@dri.edu

The notion that the kinematics of sediment transported in streams is well-represented by quasi-random motions amenable to Smoluchowski-type diffusion was first proposed by Hans Albert Einstein at his renowned father's suggestion. Since then, there have been attempts to adapt formalisms of diffusion and anomalous diffusion developed for thermodynamic systems to the start-and-stop and spatially variable behavior of sediment transport. New high-resolution measurements of sediment particle motions in laboratory flumes indicate that the mean squared displacement of tracer particles , when treated as a plume reflects a nonlinear increase in the variance in hop distances with increasing travel time. Ensemble calculations of MSD indicates a transition from correlated random walks to normal diffusion. Normal behavior also is reflected in the particle velocity autocorrelation function. Spatial variations in particle entrainment produce a flux from sites of high entrainment toward sites of low entrainment; thus, an entrainment form of flux and continuity equations are used for describing statistically expected transport behavior.

Session 3 / **163**

Progressive quenching

Author: Ken Sekimoto[1]

Co-authors: Bruno Ventejou [2]; Michael Etienne [2]

[1] *Univ. Paris-Diderot & ESPCI*

[2] *ESPCI*

Corresponding Author: ken.sekimoto@espci.fr

We will describe the basic idea and some applications of the processes when the system's degrees of freedom are progressively quenched. This work has been done in collaboration with Bruno Ventejou and Michael Etienne (paper in preparation).

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Negative mobility of a Brownian particle in the strong damping regime

Author: Aleksandra Slapik[1]

Co-authors: Jakub Spiechowicz [1]; Jerzy Łuczka [1]

[1] *University of Silesia*

Corresponding Author: aleksandra.slapik@smcebi.edu.pl

We study impact of inertia on directed transport of a Brownian particle under non-equilibrium conditions: the particle moves in a one-dimensional periodic and symmetric potential, is driven by both an unbiased time-periodic force and a constant force, and is coupled to a thermostat of temperature T. Within selected parameter regimes this system exhibits negative mobility, which means that the particle moves in the direction opposite to the direction of the constant force. It is known that in such a setup the inertial term is essential for the emergence of negative mobility, which cannot be detected in the limiting case of overdamped dynamics. We analyse inertial effects and show that negative mobility can be observed even in the strong damping regime. We determine the optimal dimensionless mass for the presence of negative mobility and reveal three mechanisms standing behind this anomaly: deterministic chaotic, thermal noise induced and deterministic non-chaotic. To the best of authors knowledge the last origin has never been reported before. It may provide guidance to the possibility of observing negative mobility for strongly damped dynamics which is of fundamental importance from the point of view of biological systems, all of which operate in fluctuating environments.

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Asymptotic behaviour of time averages for non-ergodic Gaussian processes

Author: Jakub Slezak[1]

[1] *Wroclaw University of Science and Technology*

Corresponding Author: jakub.slezak@pwr.edu.pl

We study the behaviour of time-averages for stationary (non-ageing), but ergodicity-breaking Gaussian processes using their representation in Fourier space. We provide explicit formulas for various time-averaged quantities, such as mean square displacement, density, and analyse the behaviour of time-averaged characteristic function, which gives insight into rich memory structure of the studied processes. Moreover, we show applications of the ergodic criteria in Fourier space, determining the ergodicity of the generalised Langevin equation's solutions.

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Abnormal behavior of rupture force distribution in PEI/SiO_2 system

Authors: Ewa Gudowska-Nowak[1]; Jakub Barbasz[2]; Kamila Sofinska[2]; Michał Cieśla[1]

[1] *M. Smoluchowski Institute of Physics, Jagiellonian University, Kraków, Poland*

[2] *Jerzy Haber Institute of Catalysis and Surface Chemistry Polish Academy of Sciences, Kraków, Poland*

Corresponding Author: ncsofins@cyf-kr.edu.pl

Understanding the dynamic properties of interacting molecules is an important issue in the field of designing micro and nano drug carriers or transfection systems. One of the most powerful research methods of these properties is dynamic force spectroscopy that allows to determine the interactions strength between single molecules, the local Young's modules or the energy landscapes. This technique enables also to explore the dynamic properties in the interacting proteins or polymer molecules systems. The dynamic force spectroscopy measurements derive the distributions of locally determined parameters which are analyzed based on models described in the literature, i.e. Bell-Evans model, Dudko, Hummer and Szabo model. Theoretical interpretation of experimental results is complex because of the wide distributions of measured forces for the multiple repetition of the experiment even for fixed rupture speed. At the same time there is a dependence of the rupture force on the rupture rate.

The results of rupture forces obtained for PEI / SiO_2 system were interpreted based on theoretical models of rupturing the interactions in the individual particles that are available in the literature. The general characteristics of results distributions obtained for the PEI-silica are consistent with existing models (narrowing of histograms with the increasing rate of the rupture speed, i.e. with the

increase of the rupture force in time). However, none of the models describe accurately the measured distributions. Regardless of whether the Bell-Evans or HSD (Hummer, Szabo Dudko) models were used, it was not possible to obtain asymmetric, heavy-tailed distributions of rupture forces. It suggests that the rupture in such system cannot be reduced to the model describing a single particle overcoming a constant energy barrier. It is possible that the proper model of PEI - SiO_2 interaction should include interactions between larger groups of particles as well as fluctuation of an interaction potential that keeps a system together.

Session 4 / **107**

Intermediate asymptotics and aging phenomena in anomalous transport by flows.

Author: Igor Sokolov[1]

Co-authors: Alexander Nepomnyashchy [2]; Michael Zaks [1]; Patrick Poeschke [1]

[1] *Humboldt University Berlin*

[2] *Technion Haifa*

Corresponding Author: igor.sokolov@physik.hu-berlin.de

Anomalous transport in flows is often invoked in discussion of anomalous transport phenomena as described by continuous-time random walk (CTRW) or Levy walk (LW) schemes. The first model describes the particles' transport in eddy lattices, and the model of a Levy walk interrupted by rests describes the transport in flows which consist of eddies and jets. The models adequately describe the intermediate-time dynamics of the mean squared displacement (MSD) of the transported particles from their initial positions under initial conditions corresponding starting on the separatrix between two eddies or between an eddy and a jet, and the long-time dynamics for any initial condition, when the initial conditions are already forgotten.

Both random walk models lead to non-stationary dynamics on intermediate times, and exhibit aging phenomena. It is sometimes assumed that the corresponding models also can describe aging in flows. The aging phenomena in random walk schemes are connected with the walker's behavior during the very first step after the beginning of the observation, and assume that this dynamics is trivial (being at rest in CTRW, or either being at rest or moving along straight line in the interrupted LW) while the dynamics during the capturing periods in a flow is essentially quite complex and corresponds to rotations around elliptic points of eddies or oscillations in jets.

We concentrate on the MSD of the transported particles from their initial positions, and discuss in detail the aging dynamics of MSD in flows. We show that the time-evolution of the MSD depends strongly on initial conditions, that simple CTRW / LW-dynamics only describes the intermediate-time behavior of the initial conditions discussed above, and that several other regimes
(including superdiffusion or oscillations) are possible. Even in the case when simplified models correctly describe the intermediate time behavior of MSD when starting on the separatrix, they fail to describe the aging behavior of the MSD even in this case. We give the theoretical discussion of all theses issues, and illustrate our points by results of massive numerical simulations of the system.

Session 2 / **130**

Mesoscopic and metastable quantum systems

Author: Bernardo Spagnolo[1]

[1] *University of Palermo*

Corresponding Author: bernardo.spagnolo@unipa.it

We shortly review the transient dynamics of mesoscopic systems, such as Josephson junctions, in noisy environments. The role of noise induced solitons and breathers on the mean switching time from the superconducting metastable state to the resistive state, in the presence of an external noise source modeled by α-stable Lévy distributions, will be outlined.
Thereafter, the dissipative dynamics of a particle moving in a strongly asymmetric double well potential, interacting with a thermal bath will be considered. Common wisdom is that quantum fluctuations enhance the escape rate from metastable states in the presence of dissipation. We show that dissipation can enhance the stability of a quantum metastable system. We find that the escape time from the metastable region has a nonmonotonic behavior, with a maximum, versus the system-bath coupling, and with a minimum versus the temperature, thus producing a stabilizing effect. Therefore, as the temperature increases, an enhancement of the escape time is observed, increasing the stability of the metastable state. These results shed new light on the role of the environmental fluctuations in stabilizing quantum metastable systems.
We will show then, how the combined effects of strong Ohmic dissipation and monochromatic driving affect the stability of a quantum system with a metastable state. We find that, by increasing the coupling with the environment, the escape time makes a transition from a regime in which it is substantially controlled by the driving, displaying resonant peaks and dips, to a regime of frequency-independent escape time with a peak followed by a steep fall off. The quantum noise enhanced stability phenomenon is observed in the system investigated. Resonant activation, the presence of a minimum in the mean escape time, occurs when the time scale of the modulations is the same as the characteristic time scale of the system's dynamics. The simple quantum system considered displays as well the general features that at slow modulations the mean escape time is dominated by the slowest configuration assumed by he system, while at fast modulations the escape dynamics is determined by the average configuration.

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Session 3 / **170**

Where are we with the understanding of a collective dynamics of quasi-periodically perturbed particles?

Author: Aneta Stefanovska[1]

[1] *Physics Department, Lancaster University*

Corresponding Author: aneta@lancaster.ac.uk

Marian Smoluchowski provided an explanation of the Brownian motion of particles. The equation for a particle's displacement in space that he proposed in 1906 provided an important basis for the theory of stochastic processes. This initiated the whole new field of stochastic dynamics that blossomed during the last century. In this talk we will discuss what happens to the particles if external deterministic forces are continuously imposed on them, and how a collective dynamics emerges to describe particles under external forcing.

The time-varying, non-autonomous, dynamics that emerges under external forcing has been detected in living, as well as man-made, systems. Currently, however, non-autonomous dynamics is commonly considered easy to deal with - either by transforming it into autonomous dynamics, for which an abundance of tractable analytic tools is available, or by considering it as belonging to the class of stochastic systems where, again, numerous analytic approaches exist.

In the talk, we will argue that there is a need for a theory of a new class of non-autonomous systems with time-varying dynamics due to external forcing. We will first present examples of non-autonomous dynamics measured from biological cells, the cardiovascular system and the brain, as well as from experiments with electrons on the surface of liquid helium.

Then, we will review briefly the existing numerical methods for the detection and analysis of non-autonomous dynamics from data. In the third part of the talk, we will summarise our current work on non-autonomous dynamics when the external perturbation is of quasi-periodic origin, arguing that most of the challenging problems still remain unsolved and that our better understanding of non-autonomous, finite-time dynamics could make a similarly significant contribution to that of Smoluchowski more than 100 years ago, thereby advancing our understanding of nature in general.

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Session 9 / **7**

The quantum first detection problem: from the energy spectrum to the detection probabilities

Author: Felix Thiel[1]

Co-authors: David A. Kessler [1]; Eli Barkai [1]

[1] *Bar-Ilan University*

Corresponding Author: thiel@posteo.de

We consider the question of when a quantum system initially prepared in state A first "arrives" in state B, i.e. the first arrival problem in quantum physics.
To determine the arrival, the observer attempts to detect the system stroboscopically with fixed period via a projective measurement.
The time of the first successful detection attempt is the first detection time.
The corresponding probability of the event is the first detection probability.
For systems with a continuous energy spectrum, this quantity can be expressed in terms of the spectral measure of the evolution operator (which is related to the density of energy states).
This allows us to present an exact formula for the total probability of detection and to derive the long-time asymptotic behavior of the first detection probabilities.
It is shown that the latter decays like a power law with superimposed oscillations.
The exponent of the power law is determined by the spectral (or fracton) dimension of the spectral measures.
The total probability of detection is always less than unity.

Session 12 / **125**

Individual and network heterogeneity in agent-based models

Author: Raul Toral[1]

[1] *IFISC*

Corresponding Author: raul@ifisc.uib-csic.es

Most applications of Statistical Mechanics methods to agent-based models make assumptions that aim at a simplification of the mathematical treatment and which are reasonable, or well established, in other applications of the field. Amongst others, we can cite the assumption of the thermodynamic limit and the assumption that there is a high degree of homogeneity amongst the agents. This is certainly not true in most cases: the number of agents is never close to the Avogadro number and the dispersion in the individual features of agents is an unavoidable nature of the system. In this talk I will discuss some difficulties associated to the existence of such a heterogeneity and the mathematical tools that can be used to achieve analytical results. As an example, I will consider in detail both network and parametric heterogeneity in Kirman's model for herding behavior in financial markets. Stylized facts of financial markets (fat tails, volatility clustering) has been proposed as an emergent phenomenon of interactions among traders. One of the simplest agent-based models capable of reproducing these statistical properties is the one proposed by Kirman. The fundamental aspect of the model is that agents change opinion based on the proportion of neighbor agents holding it. The effect of network structure on the results of the model is also addressed with recent analytical tools known as heterogeneous mean field approximations. This approach suggests that the dynamics in an heterogeneous degree network is equivalent to the usual all-to-all approximation with an effective system size $N_{\text{eff}} = N\mu_1^2/\mu_2$, where μ_k is the k-th moment of the degree distribution. This implies that highly heterogeneous degree networks are characterized by a low effective population number. Intuitively, only highly connected agents play an important role in the dynamics and the number of those agents is measured by this effective population number. Taking into account that most real networks are highly heterogeneous with power-law degree distributions, one concludes that the effect finite-size fluctuations is non-trivial and must be studied in detail for each specific type of network.

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Entropy-based analysis of the surface electromyography signals

Author: Paulina Trybek[1]

Co-authors: Lukasz Machura [1]; Michal Nowakowski [2]

[1] *Silesian Center for Education and Interdisciplinary Research, University of Silesia, Chorzow, Poland*

[2] *Jagiellonian University School of Medicine, Krakow, Poland*

Corresponding Author: paulina.trybek@smcebi.edu.pl

Physiological systems are characterized by high dynamical complexity, which is conditioned by their ability to adapt in incessantly changing environment. Loss of such complexity can be related with occurring the pathological state, what has been gained widespread use in biomedical signal analysis.
Among the nonlinear methods that take into account an internal structure of the signal together with the insight into its complexity over a range of scales, the entropy of series has found wide application.
Based on sample entropy parameter (SampEn) which has been successfully investigated in the context of data characterized by the low signal to noise ratio, we present the application of Multiscale Entropy method (MSE) to the surface electromyography signals(sEMG).

The usefulness of that approach has been illustrated by examining the muscle activity of external anal sphincter during multimodal rectal cancer treatment which mainly involved surgery and radiotherapy. Both, the specific values of the entropy measure and the dependence on the time scale were analyzed due to the factors such as time period after surgery and the use of radiation therapy. Also the contraction and relaxation state in conjunction with the different levels of signal acquisition were considered separately.

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Session 9 / **129**

Heterogeneous continuous time random walk on graphs

Author: Liubov Tupikina[1]

Co-author: Denis Grebenkov [2]

[1] *Ecole Polytechnique*

[2] *CNRS*

Corresponding Author: lyubov78@gmail.com

Solute transport and, particularly, diffusion of particles in porous media is a long standing problem [1].
The general random walks framework has been shown to describe quantitatively the anomalous transport patterns frequently observed in fractured and heterogeneous porous media [2]. One of the major conceptual difficulties consists in a very broad range of time and length scales in the dynamics [3]
that prohibits using conventional theoretical approaches or numerical simulation methods.

To
overcome this problem and bridge various scales, we present a new model, Heterogeneous Continuous Time Random Walk model (HCTRW) and suggest to represent a porous medium by an

equivalent "porous graph" and then to model the complex dynamics of a particle in the porous medium by a continuous time random walk (CTRW) on that porous graph. The graph structure accounts for the inter-connectivity of pores, whereas their geometric properties (shapes of pores and of connectivity regions) are, to some extent, captured through the CTRW characteristics, hence connecting the topological and dynamical properties of the system.
In our CTRW approach, the space and time characteristics of individual jumps on a graph are coupled that requires developing new theoretical tools. We present several preliminary results on the long-time asymptotic behavior of a particle on a porous graph. To validate the proposed coarse-graining scheme, we compare the asymptotic behavior of the CTRW on a porous graph with the original continuous dynamics in several models of porous media. In particular, we investigate how topology of a graph (which would correspond to i.e. the interconnectivity of pores) can affect the long-time behavior of HCTRW.

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Stronger selection can slow down evolution driven by recombination on a smooth fitness landscape

Author: Masahiko Ueda[1]

Co-authors: Kunihiko Kaneko [1]; Nobuto Takeuchi [1]

[1] *Department of Basic Science, The University of Tokyo*

Corresponding Author: ueda@complex.c.u-tokyo.ac.jp

Stronger selection implies faster evolution—that is, the greater the force, the faster the change. This apparently self-evident proposition, however, is derived under the assumption that genetic variation within a population is primarily supplied by mutation (i.e. mutation-driven evolution). Here, we show that this proposition does not actually hold for recombination-driven evolution, i.e. evolution in which genetic variation is primarily created by recombination rather than mutation. By numerically investigating population genetics models of recombination, migration and selection, we demonstrate that stronger selection can slow down evolution on a perfectly smooth fitness landscape. Through simple analytical calculation, this apparently counter-intuitive result is shown to stem from two opposing effects of natural selection on the rate of evolution. On the one hand, natural selection tends to increase the rate of evolution by increasing the fixation probability of fitter genotypes. One the other hand, however, it tends to decrease the rate of evolution by decreasing the chance of recombination between immigrants and resident individuals. As a consequence of these opposing effects, there is a finite selection pressure maximizing the rate of evolution; hence, the change" depends on theforce" non-monotonically.

Stochastic advection-reaction-diffusion model for phytoplankton populations in a 2D spatial domain

Author: Davide Valenti[1]

[1] *Department of Physics and Chemistry, University of Palermo*

Corresponding Author: davide.valenti@unipa.it

Phytoplankton lies at the base of the food chain of seas and oceans, and it is responsible for about 80% of the total *chlorophyll a*. As a consequence, phytoplankton determines the trophic structures of marine ecosystems, while influencing the total abundance and the spatial distributions of marine biological species, e.g. fish populations. Thus the study of spatio-temporal dynamics of phytoplankton populations and the development of models which predict the trend of primary production become of paramount importance to understand and forecast the dynamics of biological species within marine ecosystems.
Here it is presented a two-dimensional advection-reaction-diffusion model to describe the dynamics of four phytoplankton populations in a real ecosystem located in the Channel of Sicily (South Mediterranean Sea). Light intensity and nutrient concentration represent the limiting factors for the phytoplankton growth. Specifically, due to the characteristics of the marine ecosystem analyzed, i.e. a transect consisting of twelve marine stations between Cape Passero (Sicily) and Misurata (Libya) [1], the limiting nutrient component is phosphorus.
Phytoplankton abundances are first obtained by solving numerically a system of deterministic partial differential equations and then converted *chlorophyll a* concentrations [2], whose spatial distributions are compared with those obtained from field data collected in the twelve marine stations [3]. Statistical checks based on the chi-square test indicate a good agreement between theoretical and experimental distributions of *chlorophyll a* concentration.
Deterministic models however can not fully describe the nonlinear dynamics of a real ecosystem continuously exposed not only to deterministic but also to random perturbations coming from the environment. To take into account the random fluctuations of the environmental variables, the deterministic model is modified by inserting in the equations Gaussian noise sources [4]. As confirmed by checks based on the chi-square test, the distributions of *chlorophyll a* concentration obtained by the stochastic model fit the field data better than those calculated by the deterministic model.
It is worth noting that in this study real values for physical and biological variables were used. Specifically, the analysis exploits hydrological and nutrients data acquired in situ, including intraspecific competition for limiting factors.
The study and the results discussed here indicate the effectiveness of this approach for reproducing real spatial distributions of *chlorophyll a* concentration. Moreover we note that the stochastic advection-reaction-diffusion model presented in this work can be extended to different marine ecosystems and used as a global model to forecast eventual decreases in the abundance of primary production and to prevent the consequent decline of fish species.

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Quantum thermostatted disordered systems and sensitivity under compression

Authors: Rondoni Lamberto[1]; Tommaso Vanzan[2]

[1] *Politecnico di Torino*

[2] *University of Geneva*

Corresponding Author: tommaso.vanzan@unige.ch

We consider a one-dimensional quantum system with off diagonal disorder, consisting of a sample of conducting regions
randomly interspersed within potential barriers.
Results mainly concerning the large N limit are presented and it is shown that the disordered model converges to the periodic case as the number of barriers increases, with a rate of convergence which depends on the disorder degree. In particular, the effect of compression on the transmission coefficient is investigated. Compression always leads to a decrease of the transmission coefficient which may be exploited to design nano-technological sensors. Effective choices for the physical parameters to improve the sensitivity are provided and eventually large fluctuations and rate functions are analysed, which can be used to revel the compression state of the system.
Moreover, a numerical method to simulate such a system, for a physically relevant number of barriers, is proposed.

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The (random) matrix reloaded. Old tricks for new dogs - and return

Author: Pierpaolo Vivo[1]

[1] *King's College London*

Corresponding Author: pierpaolo.vivo@kcl.ac.uk

Matrices with random entries - much like cats - enjoy several lives. Studied in one context, they usually prove more useful in another, giving rise to more and more baffling challenges and unexpected twists as time goes by. But, the field of random matrices is also plagued by false myths, inaccurate historical accounts, and true gems that - while jealously kept from our colleagues - would certainly deserve a better fate. I will give a cheerful account of the 'old tricks' of the trade in the occasion of the 89th birthday of Random Matrix Theory, and how well they assist us with a few - nasty - 'new dogs'. Also, how technical advancements in the field have made it possible - at long last - to make significant progresses in our understanding of old problems. In the course of my talk, I will likely get many cats out of the bag - as progress in science often relies on not letting sleeping dogs lie!

Session 5 / 31

Mechanical interactions affect biological evolution in bacterial colonies

Author: Bartlomiej Waclaw[1]

[1] *University of Edinburgh*

Corresponding Author: bwaclaw@staffmail.ed.ac.uk

Bacterial conglomerates such as biofilms and microcolonies are ubiquitous in nature and play an important role in industry and medicine. In contrast to well-mixed cultures routinely used in microbial research, bacteria in a microcolony interact mechanically with one another and with the substrate to which they are attached. Here we use a computer model of a microbial colony of rod-shaped cells to investigate how physical interactions between cells determine their motion in the colony and how this affects biological evolution. We show that the probability that a faster-growing mutant "surfs" at the colony's frontier and creates a macroscopic sector depends on physical properties of cells (shape, elasticity, friction). Although all these factors contribute to the surfing probability in seemingly different ways, they all ultimately exhibit their effects by altering the roughness of the expanding frontier of the colony and the orientation of cells. Our predictions are confirmed by experiments in which we measure the surfing probability for colonies of different front roughness. Our results show that physical interactions between bacterial cells play an important role in biological evolution of new traits, and suggest that these interaction may be relevant to processes such as de novo evolution of antibiotic resistance.

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Entropy facilitated transport of potassium ions through Kv 1.2 channels

Author: Agata Wawrzkiewicz-Jalowiecka[1]

Co-author: Zbigniew Grzywna [1]

[1] *Silesian University of Technology, Faculty of Chemistry*

Corresponding Author: agata.wawrzkiewicz@polsl.pl

We analyze how changes of channel pore geometry during membrane depolarization can influence transport properties of Kv 1.2 channel protein. Spatial confinements of the channel give rise to entropic barriers which effectively influence its ability to transport the potassium ions through the membrane.
First, on the base of structures of the channel in an open state at membrane depolarization (full voltage activation of the channel) and hyperpolarization (implying low activity of the channel) we calculate the difference in entropy between fully voltage-activated and resting state of the channel. The obtained result indicates that voltage-activation is an entropy-driven process.
Second, we describe the differences in characteristics of K+ transport through the channel pore at different voltages basing on the results of random walk simulations in entropic and electric potentials.

Session 6 / **179**

An anomalous diffusion approach to stochastic modeling for single molecule tracking of receptors and proteins at cell surface

Author: Aleksander Weron[1]

Co-author: Krzysztof Burnecki [2]

[1] *Hugo Steinhaus Center, Faculty of Pure and Applied Mathematics, Politechnika Wrocławska*

[2] *Wroclaw University of Science and Technology*

Corresponding Author: aleksander.weron@pwr.edu.pl

The Nobel Prize in Physiology or Medicine 2009 was awarded for the discovery of how chromosomes are protected by telomeres and the enzyme telomerase. The Nobel Prize in Chemistry 2012 was given for studies of G-protein-coupled receptors and the Nobel Prize in Chemistry 2014 was presented for the development of superresolved fluorescence microscopy. Definitely, the research behind these Nobel Prizes - awarded within a short few years period - have caused a dramatic increase of experimental and theoretical achievements in the study of living cells around the world.

Ultimately the accessibility of quantitative data prompted many statistical physicists and applied mathematicians to turn their attention to the study of single biological cells and the physiological processes running off therein. For example, G protein-coupled receptors mediate the biological effects of many hormones and neurotransmitters and are major pharmacological targets, [1-4]. However, how receptors and G proteins interact and couple at the plasma membrane is not well understood.

A phenomenon observed in recent single-molecule experiments is anomalous diffusion, which largely departs from the classical Brownian diffusion theory since the mean-squared displacement (MSD) is nonlinear. The most popular theoretical models that are commonly employed are: continuous-time random walk (CTRW), fractional Brownian motion (FBM), fractional Langevin equation (FLE) and autoregressive fractionally integrated moving average (ARFIMA).

Using single-molecule imaging data one can visualize motion of individual receptors and G proteins at the surface of living cells [2]. Here, we provide a detailed anomalous diffusion classification based on MSD analysis [5] for some exemplary experimental data from [2].

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Kinetic equation for Smoluchowski's diffusion

Author: Ryszard Wojnar[1]

[1] *Instytut Podstawowych Problemów Techniki Polskiej Akademii Nauk*

Corresponding Author: rwojnar@ippt.pan.pl

Smoluchowski's diffusion, [1], it is a diffusion in an external field is studied, and a general kinetic equation valid within the framework of classical statistical mechanics is found.

We apply Stecki's projection operator method, [2], to obtain a kinetic equation for an auxiliary distribution function f(k,v_1,t). This function yields the intermediate scattering function I_s(k,t), which is a Fourier transform of van Hove's function G_s(r,t). The function G_s(r,t) gives the probability of finding in a equilibrium system a given (marked) particle at (r,t), if it was known to be at the position r=0 at the time t=0. A kinetic equation of the convolution type for the time evolution of the distribution function f(k,v_1,t) is given.

Diffusion problems studied in the time scale comparable with time of particles collision lead to kinetic equations which for step-wise potentials are functional equations in the velocity space.

We start, as usually in statistical physics from Liouville's theorem, which is a key theorem in classical statistical and Hamiltonian mechanics. The gas is composed of N particles. We pay a particular attention to Lorentz' gas with N-1 immovable particles-scatterers, between which a light particle number 1 is moving, and to Brownian diffusion (one heavy–marked particle among N-1 light particles). The second case is a natural generalization of Smoluchowski's equation.

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Brownian dynamics simulation of protein-polyelectrolyte particle formation and growth

Author: Miao Yu[1]

Co-authors: Ahmad Sediq [2]; Geert-jan Witkamp [1]; Hayley Every [3]; Peter Verheijen [1]; Reza Nejadnik [2]; Wim Jiskoot [2]

[1] *Department of Biotechnology, Delft University of Technology, Delft, the Netherlands*

[2] *Division of Drug Delivery Technology, Cluster BioTherapeutics, Leiden Academic Centre for Drug Research (LACDR), Leiden University, Leiden, the Netherlands*

[3] *FeyeCon Development & Implementation B.V., Weesp, the Netherlands*

Corresponding Author: m.yu@tudelft.nl

The interaction between protein and polyelectrolytes is relevant for the development of protein drug delivery systems [1]. The formation and growth of protein-polyelectrolyte complexes has been monitored experimentally by nanoparticle tracking analysis (NTA) and flow imaging microscopy (MFI) [2]. Although Smoluchowski's theory was able to describe the agglomeration in this system, it can be expected that if systems become more complex (for instance when starting with size distributions instead of a single particle size), finding the analytical solution may not be easy. Therefore we develop here a simulation environment that allows explicit size dependent particle properties to be loaded in a Brownian motion based agglomeration process.

A direct collision (DC) simulation was developed focusing on the perikinetic particle agglomeration. In the simulation, particles are displaced stochastically in short time steps where the displacement distance is shorter than their diameters. Whenever two particles are close to each other within the distance of effective collision diameter, a merge of the two particles is assumed to take place. In order to lift the simulation efficiency, the DC simulation always starts with hundreds of particles in a

mini-volume (about 1E-14 – 1E-13 m3) followed by step-by-step expansion into larger volumes while maintaining the particle number concentration constant (typically about 1E15 particles/m3).

The DC simulation was validated through comparisons with analytical solutions of Smoluchowski's model, and with the modelling results on gold particles described in Smoluchowski's own paper [3]. It was found that for the given systems a short displacement distance of maximally ≈1/4 of the particle diameter was necessary for a good fit.

The DC simulation was applied to experimental data on protein-polyelectrolyte particle growth. The DC simulation started with an initial particle concentration of 1.23E15/m3 as reported [2] after 1 min of the mixing of protein and polyelectrolyte. From the fit of the particle size envelope a ratio of effective particle collision radius versus the real particle radius was calculated to be 0.2-0.5. This value is much lower than that was reported by Smoluchowski [3] for gold particles. This short effective collision distance for proteins compared with the real radius of the particle made a shorter displacement distance (≈1/10 of the particle size) in the simulation necessary.

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Session 13 / **99**

Eliminating ensembles from equilibrium statistical physics: Maxwell's demon, Szilard's engine, and thermodynamics via entanglement

Author: Wojciech Zurek[1]

[1] *Los Alamos*

Corresponding Author: whz@lanl.gov

A system in equilibrium does not evolve: time independence is its telltale characteristic. However, in Newtonian physics microstate of an individual system (a point in its phase space) evolves incessantly in accord with its equations of motion. Ensembles were introduced in XIX century to bridge that chasm between continuous motion of phase space points in Newtonian dynamics and stasis of thermodynamics: While states of individual classical system inevitably evolve, a phase space distribution of such states – an ensemble – can be time-independent. I show that entanglement (e.g., with the environment) can yield time-independent equilibrium in an individual quantum system. This allows one to eliminate ensembles – an awkward stratagem introduced to reconcile thermodynamics with Newtonian mechanics – and use individual system interacting with its heat bath to represent equilibrium and to elucidate the role of information and measurements in physics. Thus, in our quantum Universe one can practice statistical physics without ensembles. I illustrate classical difficulties and the need for ensembles with Szilard's engine, and show that in a similar quantum engine a single system entangled with the environment is enough. The role of Maxwell's demon (which in this quantum context resembles Wigner's friend) is also discussed.

Griffiths phases on a large human Open Connectome network

Session 0 / **194**

Opening