37th M. Smoluchowski Symposium on Statistical Physics

Monday, 16 September 2024 - Wednesday, 18 September 2024 Faculty of Physics, Astronomy and Applied Computer Science; Jagiellonian University



Book of Abstracts

ii

Contents

Dissipation bounds precision of current response to kinetic perturbations	1
Changeover phenomenon in randomly colored Potts models	1
Radiation adaptive response: the biophysical phenomenon and its theoretical description	2
Information entropy calculations for mutating viruses	2
Application of Avrami phase transition model to cellular carcinogenesis	3
Effective mass approach to memory in non-Markovian systems	3
Heat exchange at strong coupling: An example	3
Nonergodic Brownian Oscillator: Relaxation and response properties	4
Disorder-induced anomalous mobility enhancement in confined geometries	4
Critical Fluctuations at Finite-Time Dynamical Phase Transition	5
Giant enhancement of free particle transport induced by active fluctuations	5
The distribution of first passage times of random walks on random regular graphs \ldots	6
Inference of developmental processes and gene expression programs from single-cell mul- timodal data.	7
Analysing phase space of heterogeneous anomalous diffusion	7
Delayed interactions in active matter models	8
Comparison of methods of functional connectivity estimation in investigation of diurnal changes in working memory performance	8
A Numerical Study on the Diffusion Behavior of an Anisotropic Molecule in Cylindrical and Trapezoidal Channel	9
The Price-Pareto-Gini model for evolving networks	9
Conditional approach to weak fluctuation correlation in nonequilibrium complex systems	10
Study of micelle formation in water by molecular dynamic simulations and thermodynamic approach	10
Thermodynamic Uncertainty Relation in Systems with Inertia	11

Force from coarse graining nonequilibrium degrees of freedom	11
Hydrodynamics of pulsating liquids	12
Spinning Colloid in viscoelastic fluid	12
New class of multimodal Turing patterns	13
Modeling mutations, drift, selection, and genome transformations in carcinogenesis	13
Restoring the Fluctuation–Dissipation Theorem in phase transition through a New Emer- gent Fractal Dimension	14
Multi point observables for stochastic trajectories	14
Extreme robustness of subdiffusion as described by a generalized Langevin equation	15
Tissue fluidization in developing spinal cord	15
Self-organization, Criticality and Collective Information Processing in Animal Groups .	16
Rényi Entropy of Zeta-Urns	16
Opening	17
Lévy flights and Lévy walks under stochastic resetting	17

Session 7 / 1

Dissipation bounds precision of current response to kinetic perturbations

Author: Krzysztof Ptaszyński¹

Co-authors: Massimiliano Esposito²; Timur Aslyamov²

¹ Institute of Molecular Physics, Polish Academy of Sciences; University of Luxembourg

² University of Luxembourg

Corresponding Author: krzysztof.ptaszynski@ifmpan.poznan.pl

The precision of currents in Markov networks is bounded by dissipation via the so-called thermodynamic uncertainty relation (TUR) [1]. In our work [2], we demonstrate a similar inequality that bounds the precision of the static current response to perturbations of kinetic barriers. Perturbations of such type, which affect only the system kinetics but not the thermodynamic forces, are highly important in biochemistry [3] and nanoelectronics [4]. We prove that our inequality cannot be derived from the standard TUR. Instead, it implies the standard TUR and provides an even tighter bound for dissipation. We also provide a procedure for obtaining the optimal response precision for a given model.

K.P. acknowledges the financial support from project No. 2023/51/D/ST3/01203 funded by the National Science Centre, Poland.

References

[1] A. C. Barato, U. Seifert, Phys. Rev. Lett. 114, 158101 (2015)

[2] K. Ptaszyński, T. Aslyamov, M. Esposito, arXiv:2406.08361 (2024)

[3] J. A. Owen, T. R. Gingrich, J. M. Horowitz, Phys. Rev. X 10, 011066 (2020)

[4] N. Freitas, J.-C. Delvenne, M. Esposito, Phys. Rev. X 11, 031064 (2021)

Session 5 / 2

Changeover phenomenon in randomly colored Potts models

Author: Nir Schreiber¹

Co-authors: Reuven Cohen¹; Gideon Amir¹; Simi Haber¹

¹ Bar Ilan University

Corresponding Author: nir.schreiber@gmail.com

The celebrated "standard" q-state (color) Potts model, where the ferromagnetic interaction is between nearest-neighboring spins on the square lattice, is known to change its temperature-driven phase transition, from continuous to discontinuous, at some critical integer $q_c = 4$ [1,2,3]. Renormalization group theory suggests that this result should hold for other lattices or interaction content, provided that the interaction is local. There are, however, counterexamples of models with a local interaction and $q_c < 4$ [4,5].

We [6] present a new and general hybrid Potts scheme (HPS) where q_c can be manipulated, by introducing inhomogeneity to the system. More precisely, spins are chosen at random with probabilities p and 1-p, to be colored in q_0 and q colors, respectively, where $q_0 \leq q_c < q$. We show that, when HPS is applied to the standard model, for any allowed setup of spin numbers q_0, q there is a concentration p^* where the transition type of the model is changed.

Independently, a mean-field-like interaction HPS is studied. It is shown that p^* exists for this HPS. Exact expressions for the second order critical line in concentration-temperature parameter space, together with some other related critical properties, are derived.

[1] R.J. Baxter, J. Phys. C: Solid State Phys. 6, (1973).

[2] H. Duminil-Copin, V. Sidoravicius and V. Tassion, Commun. Math. Phys. 349, (2016).

- [3] H. Duminil-Copin, N. Gagnebin, M. Harel, I. Manolescu and V. Tassion, arXiv:1611.09877, (2016).
- [4] R. Tamura, S. Tanaka and M. Kawashima, Prog. Theor. Phys. 124, (2010).
- [5] N. Schreiber, R. Cohen, S. Haber, G. Amir and B. Barzel, Phys. Rev. E 100, (2019).

[6] N. Schreiber, R. Cohen, G. Amir and S. Haber, J. Stat. Mech. 2022, (2022).

Session 4 / 4

Radiation adaptive response: the biophysical phenomenon and its theoretical description

Author: Krzysztof Fornalski¹

¹ Wydział Fizyki, Politechnika Warszawska

Corresponding Author: krzysztof.fornalski@pw.edu.pl

The radiation adaptive response (or radioadaptiation) effect is a biophysical and radiobiological phenomenon responsible for e.g. the enhancement of repair processes, cell cycle and apoptosis regulation or enhancement of antioxidant production in cells / organisms irradiatied by low doses and low dose-rates of ionising radiation. Here we propose a comprehensive and complete theoretical model of radioadaptation grounded in mathematical concept of dose- and time-related probability function of the adaptive response appearance. This can be used in the context of two special cases of the adaptive response: the Raper-Yonezawa (priming dose) effect or constant low dose-rate irradiation (e.g. for high natural background). This complete theoretical approach is supported by Monte Carlo simulations and real experimental data used for model calibration and validation. Additionally, we show that the presented effect is just a special case of wider and generalized adaptation of physical systems, which can be delivered from basic laws of statistical physics, especially perturbative behaviours of far-from-equilibrium stationary states.

Poster Session and Coffee / 5

Information entropy calculations for mutating viruses

Author: Jan Ostrowski¹

Co-author: Krzysztof Fornalski¹

¹ Wydział Fizyki, Politechnika Warszawska

Corresponding Author: jan.ostrowski2.stud@pw.edu.pl

According to the well-known biophysical Single Hit Target Model, DNA chain damage, caused for instance by ionizing radiation, is purely random in nature. This presentation demonstrates that such radiation-induced DNA damage is associated with an increase in system entropy, which is characteristic of purely stochastic processes. However, it turns out that not all changes in the DNA region exhibit the same nature of change, as evolving and self-adapting systems far from thermodynamic equilibrium are characterized by a decrease in their own entropy. A good example of such systems is viruses, which have plagued humanity since the dawn of time. A few years ago, Melvin Vopson demonstrated that the informational entropy calculated for various mutations of the SARS-COV2 (COVID-19) virus decreases over time (number of mutations). This is an example consistent with Prigogine and Onsager's theory for systems far from thermodynamic equilibrium, which evolve towards a future steady state. This paper will present calculations of entropy changes for mutating viruses, using COVID, HIV, and influenza virus as examples. The decrease in entropy is observed using both classical statistical methods and Bayesian robust regression methods. Importantly, characteristic local steady states are observed for the most stable virus mutations (e.g., the Omicron

mutation for the COVID virus), and transitions between subsequent stable mutations are bifurcational in nature. This may be significant in developing methods for predicting future mutations and directions of virus evolution.

Poster Session and Coffee / 6

Application of Avrami phase transition model to cellular carcinogenesis

Author: Julianna Krasowska¹

Co-author: Krzysztof Fornalski¹

¹ Wydział Fizyki, Politechnika Warszawska

Corresponding Author: julianna.krasowska.dokt@pw.edu.pl

The nucleation and growth theory, described by the Avrami equation (also called Johnson–Mehl– Avrami–Kolmogorov equation), and usually used to describe crystallization and nucleation processes in condensed matter physics, was applied to cancer physics as Avrami-Dobrzyński Model. This approach assumes the transforming system as a DNA chain including many oncogenic mutations. Finally, the probability function of the cell's cancer transformation is directly related to the number of oncogenic mutations. This creates a universal sigmoidal probability function of cancer transformation of single cells, as observed in the kinetics of nucleation and growth, a special case of a phase transition process. The proposed model, which represents a different view on the multi-hit carcinogenesis approach, is tested on clinical data concerning gastric cancer, breast cancer and ovary cancer. Additionally, the model was tested on mice, which allows to help in the cancer risk prediction for population. The results also show that cancer transformation follows DNA fractal geometry.

Session 1 / 7

Effective mass approach to memory in non-Markovian systems

Author: Mateusz Wisniewski¹

Co-author: Jakub Spiechowicz²

¹ University of Silesia in Katowice

² Institute of Physics, University of Silesia in Katowice

Corresponding Author: wisniewski.mateuszkordian@gmail.com

Recent pioneering experiments on non-Markovian dynamics done, e.g., for active matter have demonstrated that our theoretical understanding of this challenging yet hot topic is rather incomplete and there is a wealth of phenomena still awaiting discovery. It is related to the fact that typically for simplification the Markovian approximation is employed and as a consequence the memory is neglected. Therefore, methods allowing to study memory effects are extremely valuable. We demonstrate that a non-Markovian system described by the Generalized Langevin Equation (GLE) for a Brownian particle of mass M can be approximated by the memoryless Langevin equation in which the memory effects are correctly reproduced solely via the effective mass M^* of the Brownian particle which is determined only by the form of the memory kernel. Our work lays the foundation for an impactful approach which allows one to readily study memory-related corrections to Markovian dynamics.

Session 2 / 8

Heat exchange at strong coupling: An example

Author: Alex Plyukhin¹

¹ Saint Anselm College

Corresponding Author: aplyukhin@anselm.edu

The heat exchange fluctuation theorem (XFT) by Jarzynski and Wojcik [Phys. Rev. Lett. 92, 230602 (2004)] addresses the setting where two systems with different temperatures are brought in thermal contact at time t = 0 and then disconnected at later time τ . The theorem asserts that the probability of an anomalous heat flux (from cold to hot), while nonzero, is exponentially smaller than the probability of the corresponding normal flux (from hot to cold). As a result, the average heat flux is always normal. In that way, the theorem demonstrates how irreversible heat transfer, observed on the macroscopic scale, emerges from the underlying reversible dynamics. The XFT was proved under the assumption that the coupling work required to connect and then disconnect the systems is small compared to the change of the internal energies of the systems. We examine the validity of this assumption for a specific model of the Caldeira-Leggett type, where one system is a classical harmonic oscillator and the other is a thermal bath comprised of a large number of oscillators. The coupling between the system and the bath, which is bilinear, is instantaneously turned on at t = 0and turned off at $t = \tau$. For that model, we found that the assumptions of the XFT are not satisfied for lower values of the oscillator frequency and also for smaller values of the process duration τ . In that cases the coupling work is not negligible and the average heat exchange may be anomalous in the sense that the internal energy of a hotter (colder) system may increase (decrease).

Poster Session and Coffee / 9

Nonergodic Brownian Oscillator: Relaxation and response properties

Author: Alex Plyukhin¹

¹ Saint Anselm College

Corresponding Author: aplyukhin@anselm.edu

We consider an open (Brownian) classical harmonic oscillator in contact with a non-Markovian thermal bath and described by a generalized Langevin equation. When the bath's spectrum has a finite upper cutoff frequency, the oscillator may have ergodic and nonergodic configurations. In ergodic configurations (when exist, they correspond to lower oscillator frequencies) the oscillator demonstrates conventional relaxation to thermal equilibrium with the bath. In nonergodic configurations (which correspond to higher oscillator frequencies) the oscillator in general does not thermalize, but relaxes to periodically correlated (cyclostationary) states whose statistics vary periodically in time. For a specific dissipation kernel in the Langevin equation, we evaluate explicitly relevant relaxation functions, which describe the evolution of mean values, time correlations and response properties.

One interesting effect is an unusual resonance ("quasi-resonance") which occurs for the oscillator with the critical value of the natural frequency $\omega = \omega_c$, which separates thermalizing (ergodic) and non-thermalizing (nonergodic) configurations. In that case the resonance response to an external ac force is unrestricted (despite the presence of dissipation) and increases with time sublinearly. That response can be interpreted as a resonance between the external force and the incipient localized mode.

Disorder-induced anomalous mobility enhancement in confined geometries

Authors: Dan Shafir¹; Stanislav Burov²

¹ Bar-Ilan University, Physics department, Ramat Gan, 5290002 Israel

² Bar-Ilan University

Corresponding Author: dan.shafir@live.biu.ac.il

The diffusion of particles with passage times significantly slower than regular Brownian motion is observed in various systems, such as amorphous materials, living cells and rheology. This behavior is typically attributed to trapping or waiting times that are scale-free and uncorrelated. Our work demonstrates that correlated waiting times, termed quenched disorder, can redefine our understanding of transport properties.

We show that the mobility of a driven particle anomalously depends on channel width, increasing as it grows narrower. Remarkably, this effect suggests a reduction in friction for flow as the channel constricts, opposing expectations based on regular or even anomalous transport dynamics. We further reveal that modifying geometrical constraints in the presence of quenched disorder alters the statistics of rare events, notably extremely large trapping times, resulting in surprising alterations to motion dynamics.

References

[1] D. Shafir and S. Burov, arXiv:2403.01665 (2024), (accepted to PRL).

[2] D. Shafir and S. Burov, The case of the biased quenched trap model in two dimensions with diverging mean dwell times, J. Stat. Mech. (2022) 033301.

Session 6 / 11

Critical Fluctuations at Finite-Time Dynamical Phase Transition

Authors: Jan Meibohm¹; Massimiliano Esposito²; Nalina Vadakkayil²

¹ Technische Universit⁻at Berlin

² University of Luxembourg

Corresponding Author: nalina.vadakkayil@uni.lu

We explore the critical properties of the recently discovered finite-time dynamical phase transition in the non-equilibrium relaxation of Ising magnets. The transition is characterized by a sudden switch in the relaxation dynamics and occurs at a sharp critical time. While previous works have focused either on mean-field interactions or on investigating the properties of the critical time, we analyze the critical fluctuations at the phase transition in the nearest-neighbor Ising model on a square lattice using Monte Carlo simulations. By means of a finite-size scaling analysis, we extract the critical exponents for the transition. In two spatial dimensions, the values of the exponents approach closer to those of the two-dimensional Ising universality class in the vicinity of the critical temperature.

Session 7 / 12

Giant enhancement of free particle transport induced by active fluctuations

Author: Karol Białas¹

Co-author: Jakub Spiechowicz²

¹ University of Silesia in Katowice

² Institute of Physics, University of Silesia in Katowice

Corresponding Author: karol.bialas@us.edu.pl

Active fluctuations are detected in a growing number of systems due to self-propulsion mechanisms or collisions with active environment. They drive the system far from equilibrium and can induce phenomena which at equilibrium states are forbidden by e.g. fluctuation-dissipation relations and detailed balance symmetry. Recently a paradoxical effect has been briefly communicated in which a free particle transport induced by active fluctuations in the form of white Poisson shot noise can be enormously boosted when it is additionally subjected to a periodic potential. In contrast, within the realm of only thermal fluctuations the velocity of a free particle exposed to a bias is reduced when the periodic potential is switched on. Properties of active fluctuations necessary for the transport boost to occur were identified along with different enhancement regimes emerging for distinct Poisson noise amplitude statistics. The presented mechanism is significant for understanding non-equilibrium environments such as living cells where it can explain from a fundamental point of view why spatially periodic structures known as microtubules are necessary to generate impressively effective intracellular transport. Our findings can be readily corroborated experimentally e.g. in a setup comprising a colloidal particle in an optically generated periodic potential.

Session 5 / 13

The distribution of first passage times of random walks on random regular graphs

Author: Ofer Biham¹

Co-authors: Eytan Katzav¹; Ido Tishby¹

¹ The Hebrew University

Corresponding Author: ofer.biham@mail.huji.ac.il

We present analytical results for the distribution of first passage times of random walks (RWs) on random regular graphs (RRGs) [1]. RRGs are random networks, consisting of N nodes, in which all the nodes are of the same degree $c \ge 3$ and the connections are random and uncorrelated. Starting from a random initial node i at time t = 0, at each time step $t \ge 1$ an RW hops into a random neighbor of its previous node. For an RW starting from an initial node i, the first-passage (FP) time $T_{\rm FP}$ from i to a target node j (where $j \ne i$) is the first time at which the RW visits the target node j. The first-passage time varies between different instances of the RW trajectory. The distribution of first-passage times may depend on the choice of the initial node i and the target node j. In particular, it may depend on the length ℓ_{ij} of the shortest path (also referred to as the distance) between i and j. Averaging over all possible choices of the initial node i and the target node j one obtains the distribution of first-passage times $P(T_{\rm FP} = t)$.

We distinguish between the case in which the first-passage trajectory from the initial node i to the target node j ($j \neq i$) follows the shortest path (SPATH) between i and j and the case in which it does not follow the shortest path (non-SPATH). The SPATH trajectories are characterized by the property that the subnetwork that consists of the nodes and edges along the trajectory is a tree network and the distance ℓ_{ij} between i and j in this subnetwork is the same as in the whole network. The SPATH scenario takes place mainly for pairs of nodes for which the distance ℓ_{ij} is small, while most of the first passage trajectories follow the non-SPATH scenario.

The special case in which the initial node i is also chosen as the target node (i = j) is called the first return (FR) problem. The distribution $P(T_{FR} = t)$ of first return times of RWs on RRGs was studied in Ref. [2]. The characteristic time scale of first passage processes (when i and j are not too close to each other) is of order $t \sim N$. Another important event, which occurs at much longer time scales, is the step at which the RW completes visiting all the nodes in the network. The time at

which this happens is called the cover time, which scales like $t \sim N \ln N$ [3]. More recent results for the broader class of configuration model networks will also be discussed.

[1] I. Tishby, O. Biham and E. Katzav, J. Stat. Mech (2022) 113403.

[2] I Tishby, O. Biham and E. katzav, J. Phys. A 54 (2021) 325001.

[3] I. Tishby, O. Biham and E. Katzav, J. Phys. A 55 (2022) 015003.

Session 4 / 14

Inference of developmental processes and gene expression programs from single-cell multimodal data.

Author: Marcin Tabaka¹

Co-author: Piotr Rutkowski²

¹ International Centre For Translational Eye Research, Institute of Physical Cemistry, Polish Academy of Sciences

² (International Centre For Translational Eye Research, Institute of Physical Cemistry, Polish Academy of Sciences

Corresponding Author: mtabaka@ichf.edu.pl

The recent expansion of single-cell sequencing technologies has enabled simultaneous genome-wide measurements of multiple modalities in the same single cell. The potential to jointly profile such modalities as gene expression, chromatin accessibility, proteins, or multiple histone modifications at single-cell resolution represents a compelling opportunity to study biological processes at multiple layers of gene regulation. Analysis of single-cell multimodal datasets poses significant computational challenges because each single-cell data modality is high-dimensional. The number of measured features spans from hundreds in the case of protein epitopes to hundreds of thousands for chromatin-accessible sites. The multiple modalities profiled correspond to consecutive stages of gene expression, from its regulation by modifying chromatin architecture and engaging transcription-initiation proteins to the synthesis of mRNA and protein molecules. Thus, all modalities need to be modeled simultaneously to analyze and visualize multimodal data. I will present recently developed machine learning methods in our laboratory for (i) visualization and exploration of developmental processes with diffusion-based approaches, and (ii) inference of gene regulatory and expression programs leveraging topic modeling approaches.

Session 6 / 15

Analysing phase space of heterogeneous anomalous diffusion

Authors: Jakub Ślęzak¹; Joanna Janczura²

Co-authors: Diego Krapf ³; Ralf Metzler ⁴

- ¹ Wroclaw University of Science and Technology
- ² Wrocław University of Science and Technology
- ³ Colorado State University
- ⁴ University of Potsdam

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

Anomalous diffusion is often observed in complex environments which are inherently heterogeneous. This is expected in biological media, where variability often applies to the traced particles themselves as well as their immediate surroundings, which is theorised to locally affect their motions through transient associations. As a result, the dynamics can be non-ergodic and the description of the effective parameters describing anomalous diffusion must become probabilistic, an example of the doubly stochastic modelling. Due to the inherent fractionality of the anomalous diffusion, this can lead to the physical units of the parameters being estimated and uncertain, a pathological situation. Properly analysing features of the sample phase space under these conditions requires taking into account appropriate parameter gauge and behaviour of the joint estimators.

Poster Session and Coffee / 16

Delayed interactions in active matter models

Author: David Voráč¹

Co-authors: Artem Ryabov²; Viktor Holubec²

¹ Charles University, Prague

² Charles University

Corresponding Author: david.vorac@mff.cuni.cz

Almost universally, individual agents in collectives of **active particles** require time to examine their surroundings and form an appropriate response. Examples of when **perception and actuation delays** significantly affect system dynamics can be found in living organisms, robotic collectives, communication networks, and cellular processes like biopolymer assembly and migration. Still, theoretical descriptions of these systems often neglect the delays for mathematical simplicity. In particular, formulating a field theory of many-body systems interacting with time delay is an open problem.

Here, we investigate the applicability of **spin-wave approximation** to particle active matter models featuring delays. These models include the *Vicsek* and the more recent *Inertial Spin Model* (ISM), with the former neglecting and the latter accounting for orientational inertia. Our work introduces two levels of spin-wave approximation: discrete network and the continuum limit. The Vicsek model shows a good agreement with both types of approximation, provided that local perturbations remain within certain bounds. Conversely, the ISM exhibits satisfactory agreement only at the network level. Our findings represent a step towards a comprehensive hydrodynamic theory for delayed active many-particle models.

Poster Session and Coffee / 17

Comparison of methods of functional connectivity estimation in investigation of diurnal changes in working memory performance

Authors: Jeremi Ochab¹; Marta Lotka²

¹ Institute of Theoretical Physics, Jagiellonian University, Kraków

² Doctoral School of Exact and Natural Sciences, Jagiellonian University in Kraków

Corresponding Author: marta.lotka@doctoral.uj.edu.pl

Correlation matrix estimation from functional magnetic resonance (fMRI) data presents a major challenge for a multitude of reasons, including non-stationarity of the signal and low temporal resolution, resulting in the number of variables (locations from which the signal is sampled) exceeding the number of time points. The Pearson correlation matrix is most commonly used, but likely constitutes a suboptimal choice, as in the typical fMRI setting it exhibits strong sensitivity to any noise present in the signal. Hence, comparison of alternative methods of functional connectivity estimation is the subject of this contribution. The methods compared include: sample Pearson correlation, the detrended cross-correlation coefficient, and a symmetrized variant a non-linear cross-correlation based on filtering high-amplitude events (rBeta). Additionally, Ledoit-Wolf shrinkage was applied

to each method for noise reduction.

The methods were compared in their ability to detect statistically significant differences between experimental conditions using data obtained in an fMRI experiment investigating the effects of diurnal changes on memory performance. Comparison was conducted between resting state and task performance data, experimental phases (information encoding and retrieval) and tasks based on the Deese-Roediger-McDermott paradigm: involving either linguistic processing semantically and phonetically related words, or visual processing of images of global or local similarity. The comparison focused on eigenvalues of correlation matrices. To identify eigenvalues to corresponding eigenvectors in different conditions and subjects, agglomerative hierarchical clustering of eigenvectors was performed.

All correlation matrix estimation methods besides the rBeta-based method detected statistically significant differences between experimental tasks. All methods led to detection of differences between experimental tasks, but these were not consistent with respect to the estimation method. Application of Ledoit-Wolf shrinkage led to a more consistent detection of condition differences. Several aspects of this investigation merit further attention, particularly the impact of the details of the data analysis pipeline on the results, including the eigenvector clustering algorithm applied.

Session 8 / 18

A Numerical Study on the Diffusion Behavior of an Anisotropic Molecule in Cylindrical and Trapezoidal Channel

Authors: Michal Ciesla¹; Bartłomiej Dybiec^{None}; Monika Krasowska²; Zuzanna Siwy³; Anna Strzelewicz²

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

² Silesian University of Technology

³ Department of Physics and Astronomy, University of California, Irvine, United States

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

In many biological systems and various artificial materials that map them, particles pass through nanopores and nanochannels.

Artificial single nanopores are attracting increasing attention due to their potential use in nanofluidics, sensor technology, and information processing.

In this type of research, experiments focus on properties that affect the mobility of a molecule traveling through the channel.

However, because of experimental constraints, the variations in the shape of the channel and molecules are restricted.

In this paper, we try to overcome these limitations by performing numerical experiments of passing an anisotropic sphere cylindrical molecule of various lengths and thicknesses through a fixed-size cylindrical and trapezoidal channel.

Assuming that the molecule's movement was driven by diffusion, we determined the dependence of the effective diffusion type, the first passage time, and the molecule orientation distribution on its size.

The results show that thicker molecules pass the channel slightly slower, while their lengths do not affect the passage time.

Moreover, normal diffusion was observed despite the particle size.

[1] Cieśla, M.; Dybiec, B.; Krasowska, M.; Siwy, Z.; Strzelewicz, A. Numerical modeling of an anisotropic molecule diffusion through cylindrical channel, send to Molecules

[2] Qiu, Y.; Hinkle, P.; Yang, C.; Bakker, H.E.; Schiel, M.; Wang, H.; Melnikov, D.; Gracheva, M.; Toimil-Molare, M.E.; Imhof, A.; Siwy, Z.S. Pores with longitudinal irregularities distinguish objects by shape. ACS Nano 2015, 9, 4390–439

[3] Schiel, M.; Siwy, Z.S. Diffusion and trapping of single particles in pores with combined pressure and dynamic voltage. J. Phys. Chem. C 2014, 118, 19214–1922

Session 8 / 19

The Price-Pareto-Gini model for evolving networks

Authors: Marek Gagolewski¹; Grzegorz Siudem²; Barbara Żogała-Siudem³

¹ Warsaw University of Technology, Faculty of Mathematics and Information Science

² Warsaw University of Technology

³ Systems Research Institute Polish Academy of Sciences

Corresponding Author: grzegorz.siudem@pw.edu.pl

We consider the Price model for an evolving network, i.e., a growing graph, in which, in every iteration, we add a new vertex and join its edges to the existing vertices based on a mixture of the preferential attachment rule and the purely accidental component. We derive the models' expected vertex degrees and show that they coincide with the order statistics from the Pareto type-2 distribution. Moreover, we can show that in such a dynamical system, the Gini index (a well-known inequality measure from economics) is invariant. We also present the application of the described model for modeling the real data from citation networks. Some of the results discussed were obtained in cooperation with Anna Cena, Lucio Bertoli-Barsotti, Przemysław Nowak and Maciej J. Mrowinski.

Session 2 / 20

Conditional approach to weak fluctuation correlation in nonequilibrium complex systems

Author: Yuichi Itto¹

¹ Aichi Institute of Technology, Japan; ICP, Universität Stuttgart, Germany

Nonequilibrium complex systems often exhibit a hierarchical structure of different dynamics on different time scales. The statistical nature of spatiotemporal fluctuations relevant to the dynamics is known to be of central importance for treating a wide class of such systems. Maximum entropy principle has been the crux for describing the fluctuation distribution in the literature, beyond the equilibrium systems.

Here, a conditional entropic approach [1] is developed for nonequilibrium complex systems characterized by two slow dynamics with a weak correlation between fluctuations. The conditional fluctuation distribution is found to be governed by the weak correlation in a unified way. The result is demonstrated in heterogeneous diffusion in living cells: DNA-binding proteins in bacteria [2,3], membraneless organelles in embryos [4], and beads in cell extracts [5].

References

- [1] Y. Itto, Entropy, 25, 556 (2023).
- [2] A.A. Sadoon and Y. Wang, Phys. Rev. E, 98, 042411 (2018).
- [3] Y. Itto and C. Beck, J. Royal Society Interface, 18, 20200927 (2021).
- [4] R. Benelli and M. Weiss, New J. Phys., 23, 063072 (2021).
- [5] K. Speckner and M. Weiss, Entropy, 23, 892 (2021).

Poster Session and Coffee / 21

Study of micelle formation in water by molecular dynamic simulations and thermodynamic approach

Author: Piotr Weber¹

¹ Faculty of Applied Physics and Mathematics, Gdańsk University of Technology, Gdańsk, Poland

Corresponding Author: piotr.weber@pg.edu.pl

Surfactant molecules, above a critical concentration in solution, are able to spontaneously selfassemble to form aggregates. One of these aggregates are micelles, which are used in many field of sciences and industry. In an aqueous environment, due to the amphiphilic nature of the surfactants, the micelles in the core have a hydrophobic part. Micelles comes into contact with the aqueous environment through the hydrophilic parts of the surfactants that constitute them. In hydrophobic core of micelles, it is possible to dissolve some molecules that usually dissolve very poorly in an aqueous environment. This property of micelles is crucial in the action of detergents and also in the process of drug delivery or solubilization of membrane proteins. In the context of application, the study of micelle formation is of great interest to better control their use in many applications fields.

In this work, I will use a molecular dynamics approach to simulate micelle formation for various aqueous environmental conditions and surfactant concentrations. Simulations of this process make it possible to analyze the structure of self-assembled structures and their stability, and finally to link them with thermodynamic and statistical properties.

Poster Session and Coffee / 22

Thermodynamic Uncertainty Relation in Systems with Inertia

Author: Enrique Puga Cital¹

Co-author: Viktor Holubec¹

¹ Charles University

Corresponding Author: enrique.cital@matfyz.cuni.cz

The Thermodynamic Uncertainty Relation (TUR) establishes a fundamental trade-off between the cost of driving a system and the precision of its output. While TUR has been proven for discrete systems and overdamped Brownian motion, TUR violations for more general dynamics have been recently demonstrated using elaborate models based on underdamped dynamics. In our study, we present simple models of autonomous heat engines that break the TUR in the same context, pointing out minimal conditions for this to occur.

Session 1 / 23

Force from coarse graining nonequilibrium degrees of freedom

Author: Ion Santra¹

Co-author: Matthias Krüger²

¹ University of Gottingen

² University of GOettingen

Corresponding Author: ion08santra@gmail.com

I will discuss paradigmatic examples of a tracer trapped in a harmonic potential and coupled to nonequilibrium baths: In particular, the tracer equation of motion and its relaxation function, for which this equation is averaged under an initial tracer position. For equilibrium, the tracer-bath force on average vanishes, a well known consequence of Boltzmann statistics. If tracer and bath are subject to different temperatures, the conditioned tracer-bath force is finite, and can be as large in magnitude as the force between tracer and trapping potential. For a bath particle with intrinsic memory, e.g., an active particle, even the noise felt by the bath particle takes a finite average under conditioning of the tracer. If the noise of the bath particle is non-Gaussian, the relaxation function of the tracer can be non-monotonic as a function of time.

Session 3 / 24

Hydrodynamics of pulsating liquids

Authors: Tirthankar Banerjee¹; Thibault Desaleux¹; Jonas Ranft²; Etienne Fodor¹

¹ University of Luxembourg

² Institut de Biologie ENS Paris

Corresponding Author: tirthankar.banerjee@uni.lu

Inspired by dense contractile tissues, where cells are subject to periodic deformation, we will formulate a generic hydrodynamic theory of confluent pulsating liquids. Combining mechanical and phenomenological arguments, we will postulate that the mechanochemical feedback between the local phase, which describes how cells deform due to autonomous driving, and the local density can be described in terms of a free energy. We will show that the proposed hydrodynamic theory captures the three main states emerging in its particle-based counterparts: a globally cycling state, a homogeneous arrested state with constant phase, and a state with propagating radial waves. We will show that the competition between these states can be rationalized intuitively in terms of an effective landscape and argue that waves can be regarded as secondary instabilities. Through linear stability analysis of arrested and cycling states, we will predict phase boundaries and then discuss how these are affected by fluctuations. Overall, the results will demonstrate that our minimal, yet non-trivial model can provide a relevant platform to study the rich phenomenology of a wide class of pulsating liquids.

Session 3 / 25

Spinning Colloid in viscoelastic fluid

Authors: Debankur Das¹; Niklas Windbacher²; Xin Cao³; Matthias Krüger⁴; Clemens Bechinger⁵

- ¹ University of Goettingen
- ² ETH Zurich
- ³ Shanghai Jiao Tong University
- ⁴ University of GOettingen
- ⁵ Fachbereich Physik, Universität Konstanz, Konstanz, Germany

Corresponding Author: debankur.das@uni-goettingen.de

Spinning objects moving through air or liquids experience a Magnus force, a phenomenon widely exploited in ball sports and significant in various scientific and engineering applications. Opposed to large objects where Magnus forces are strong, they are only weak at small scales and eventually vanish for overdamped micron-sized particles in simple liquids. Here we demonstrate an about one-million-fold enhanced Magnus force of spinning colloids in viscoelastic fluids. Such fluids are characterized by a time-delayed response to external perturbations which causes a deformation of the fluidic network around the moving particle.

We further develop a general theory for spinning particles in a non-Markovian bath. Without any applied force, the interplay between rotation and stochastic noise-induced local deformations leads

to enhanced diffusion. Our theory also uncovers that for a spinning particle, orthogonal displacement components are correlated. These correlations are non-local in time and exhibit properties akin to the Magnus deflection. We present experimental evidence supporting these phenomena in viscoelastic fluids

References

Memory-induced Magnus effect (Nature Physics 19,(2023))
 Xin Cao, Debankur Das, Niklas Windbacher, Felix Ginot, Matthias Kruger, Clemens Bechinger.
 Spinning Non-Markovian Brownian particle (*to be submitted*)
 Debankur Das, Niklas Windbacher, Matthias Kruger, Clemens Bechinger.

Poster Session and Coffee / 26

New class of multimodal Turing patterns

Author: Helder Larraguivel¹

Co-authors: Luciano Marcon²; Marcin Zagórski³

 1 FAIS, UJ

² Self-Organization of Biological Systems Centro Andaluz de Biología del Desarrollo Universidad Pablo de Olavide

³ Marian Smoluchowski Institute of Physics, Jagiellonian University

Corresponding Author: helder.larraguivel@uj.edu.pl

We present a new set of Turing patterns based on the superposition of multiple waves. Turing patterns are well known solutions to a set of reaction-diffusion equations. Such patterns have been studied in the context of embryo development, chemical reactions, nonlinear optics, ecology and random walks, to name a few. The main feature of systems giving rise to Turing patterns is that a stable state of reaction is destabilized when the reactants may diffuse. The system then generates a periodic solution with a dominant wavelength, which establishes the pattern. Additionally, the system provides examples of spontaneous symmetry breaking and self organization behaviour.

Turing originally discovered his results when considering two morphogen species, the chemicals used by cells in an organism to communicate and grow into a pattern during development. The values of the kinetic and diffusion parameters leading to Turing patterns are known as Turing space. The degree and the number of polynomial inequalities defining Turing space, grow rapidly with the number of morphogens. Due to this, Turing patterns for more than two or three morphogens were mostly studied numerically on a case-by-case basis.

Now, we developed a method to construct analytically a linear solution to the reaction-diffusion system for certain regions of Turing space. This linear solution corresponds to a system with a regulatory network of diffusible morphogens. By providing analytical insights into dynamics of the morphogens we are able to show the existence of new types of Turing patterns, and relate these patterns to the structure of the network. These patterns have two dominant wavelengths in the case of four morphogenes. Moreover, we explain how it is possible to have superpositions of n wavelengths for 2n distinct morphogen species. Finally, we discuss possible implications of the obtained class of multimodal Turing patterns for establishing reproducible and precise patterns in biological systems.

Session 4 / 27

Modeling mutations, drift, selection, and genome transformations in carcinogenesis

Author: Marek Kimmel¹

¹ Rice University

Corresponding Author: kimmel@rice.edu

We discuss the dynamics of major genetic forces that shape evolution of cancer cells, using mathematics of stochastic processes. A range of biological examples will serve to illustrate the methodology, including leukemias and other hematological syndromes as well as solid neoplasia, such as lung, breast and bladder cancers. The latter example will help illustrate the notion of the field effect, in which morphologically normal cells harbor mutations promoting malignant transformations. More "exotic" phenomena such as copy number variation of DNA will be invoked to understand major events in tumor timelines.

Mathematical tools include branching processes, diffusion, models of population genetics such as Wright-Fisher and Moran models, as well as the coalescent theory. This latter provides a reverse-time view of cancer evolution facilitating statistical inference. More mathematically advanced methods such as semigroup theory, will be mentioned, though not discussed in depth.

Part of the material is based on publications of the speaker and his collaborators.

Connections with medical practice and public health policies will naturally emerge from conclusions. A number of references to past and current work on the subject will be provided.

Session 6 / 28

Restoring the Fluctuation–Dissipation Theorem in phase transition through a New Emergent Fractal Dimension

Authors: Henrique Lima¹; Alex Hansen²; Edwin Mozo³; Ismael Carrasco¹; Fernando Oliveira⁴

- ¹ University of Brasilia
- ² Norwegian University of Science and Technology
- ³ University Federal Fluminense
- ⁴ Universidade de Brasília

Corresponding Author: faooliveira@gmail.com

We develop a hypothesis that the dynamics of equilibrium systems at criticality have their dynamics constricted to a fractal subspace. We relate the correlation fractal dimension associated with this subspace to the Fisher critical exponent controlling the singularity associated with the correlation function. This fractal subspace is different from that which is associated with the order parameter. We propose a relation between the correlation fractal dimension and the order parameter fractal dimension. The fractal subspace we identify has as a defining property that the correlation function is restored at the critical point by restricting the dynamics this way[1]. We determine the correlation fractal dimension of the 2d Ising model and validate it by computer simulations. We discuss growth models briefly in this context[2].

[1] MS Gomes-Filho, P de Castro, DB Liarte, FA Oliveira Entropy 26 (3), 260 (2024)

[2] Henrique A Lima, Edwin E Mozo Luis, Ismael SS Carrasco, Alex Hansen, Fernando A Oliveira, arXiv preprint arXiv:2402.10167

Session 1 / 29

Multi point observables for stochastic trajectories

Author: Matthias Krüger¹

¹ University of Göttingen

Corresponding Author: matthias.kruger@uni-goettingen.de

We investigate what can be learned from multi-point correlations of stochastic particle trajectories, i.e., correlations that relate the particle position at multiple points in time. One such observable was recently introduced as the Mean Back Relaxation [1]. We discuss its properties and the information that can be obtained from it, as, e.g., regards time reversal symmetry [2,3]. We exemplify this in model systems as well as in trajectories obtained in living or passivated cells.

[1] Accessing activity and viscoelastic properties of artificial and living systems from passive measurement, T. M. Muenker, G. Knotz, M. Krüger, T. Betz, Nat. Mat., July 2024

[2] Entropy bound for time reversal markers, Knotz, Muenker, Betz, Krüger, Front. Phys. 11:1331835 (2023)

[3] Mean Back Relaxation for Position and Densities, G. Knotz and M. Krüger, arXiv:2311.17477

Session 7 / 30

Extreme robustness of subdiffusion as described by a generalized Langevin equation.

Author: Igor Sokolov¹

¹ Humbold University at Berlin

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

More than a decade ago, I. Goychuk reported on a universal behavior of subdiffusive motion (as described by the generalized Langevin equation) in a one-dimensional bounded periodic potential [1], where the numerical findings show that the long-time behavior of the mean squared displacement is not influenced by the potential, so that the behavior in the potential, under homogenization, is the same as in its absence. This property may break down if the potential is unbounded.

Motivated by biophysical prblems, we discuss spread of subdiffusive particles in domains with solid impenetrable walls which however do not fully constraint the particle motion. Two situations are considered so far: arrays of solid obstacles, and channels of different shapes.

The discussion of periodic arrays of solid obstacles [2] reveals that the universal subdiffusive behavior at long times is not influenced by the presence of solid scatterers, whose presence influences the behavior at intermediate times only. Similarly, the simulation of subdiffusion in channels of indefinite length in x-direction of varying width, and in channels with sinusoidal midline shows that the subdiffusion in x-direction is not affected by constraints put by the channel [3], in spite of the fact that the midline of a channel might be much longer than the displacement in x-direction. The same behavior is seen in a holonomic model of a bead on a sinusoidal and more strongly meandering wires, where some analytic insights are possible.

[1] I. Goychuk, Viscoelastic subdiffusion: From anomalous to normal, Phys. Rev. E 80 046125 (2009)
[2] E.B. Postnikov, I.M. Sokolov, Subdiffusion in an array of solid obstacles, J. Phys. A: Math. Theor. 57 055002

[3] E.B. Postnikov, I.M. Sokolov, Generalized Langevin subdiffusion in channels: The bath always wins!, submitted

Tissue fluidization in developing spinal cord

Author: Marcin Zagórski¹

¹ Marian Smoluchowski Institute of Physics, Jagiellonian University

Corresponding Author: marcin.zagorski@uj.edu.pl

Session 2 / 32

Self-organization, Criticality and Collective Information Processing in Animal Groups

Author: Pawel Romanczuk¹

¹ Institute for Theoretical Biology, Department of Biology, Humboldt Universität zu Berlin

Corresponding Author: pawel.romanczuk@hu-berlin.de

Collective behavior of animals is a fascinating example of self-organization in biology. This phenomenon is believed to provide several advantages to individuals, such as facilitating exchange of social information, promoting accurate collective decisions, or affording protection from predators. It has been theorized that animal collectives should operate in a special parameter region close to a critical point [1], where various aspects of collective computations become optimal [2]. Here, we discuss the "criticality hypothesis" in the context of collective animal behavior by combining experimental data and individual-based modeling. First, we will analyze self-organized coordination of movement in Trichoplax adhaerens, one of the simplest multicellular animals devoid of a central nervous system [3]. Subsequently, we shift our focus to the collective response of fish to predators. Using a spatially-explicit schooling model, we will investigate the optimal collective response at the transition between order and disorder, and individual-level evolutionary adaptation as a mechanisms for self-organization towards criticality [4]. Finally, by combining experimental data from laboratory setting and field experiments with computational models, we will explore the criticality hypothesis in relation to so-called "startle cascades", which represent rapid escape responses propagating through fish schools, akin to the activity avalanches observed in neuronal systems [5,6].

[1] T. Mora, W. Biale, J Stat Phys 144, 268-302 (2011);

[2] P. Romanczuk, B.C. Daniels. "Phase transitions and criticality in the collective behavior of animals-self-organization and biological function." In Order, Disorder and Criticality: Advanced Problems of Phase Transition Theory, pp. 179-208. 2023.

[3] Davidescu et al, Proc Natl Acad Sci 120 (2023);

[4] P.P. Klamser, P. Romanczuk, PLoS Comp Biol 17, e1008832 (2021);

[5] W. Poel et al., Sci Adv 8, eabm6385 (2022);

[6] L. Gómez Nava et al., Nature Phys 19 (2023);

*This work was supported by the Deutsche Forschungsgemeinschaft (German Research Foundation): RO 4766/2-1 and under Germany's Excellence Strategy - EXC 2002/1 'Science of Intelligence' project-no. 390523135.

Session 8 / 33

Rényi Entropy of Zeta-Urns

Author: Zdzislaw Burda¹

¹ AGH University of Science and Technology

$Corresponding \ Author: \ zdzislaw.burda@agh.edu.pl$

Session 1 / 34

.

Opening

Author: Ewa Gudowska-Nowak¹

¹ Jagiellonian University in Kraków

Corresponding Author: ewa.gudowska-nowak@uj.edu.pl

•

Poster Session and Coffee / 36

Lévy flights and Lévy walks under stochastic resetting

Author: Bartosz Żbik^{None}

Co-author: Bartłomiej Dybiec

Corresponding Author: bartosz.zbik@student.uj.edu.pl

Escape kinetics of a stochastic process can be influenced by imposing stochastic resetting, a protocol of starting anew. We study the escape kinetics from a finite interval restricted by two absorbing boundaries in the presence of heavy-tailed, Lévy type, α -stable noise. We find that the width of the domain where resetting is beneficial depends on the value of the stability index α determining the jump length distribution. The domain is narrower for heavier (smaller α) distributions in comparison to lighter tails. Additionally, we explore connections between Lévy flights (LF) and Lévy walks (LW) in presence of stochastic resetting. In the domain characterized by a finite mean jump duration/length, with increasing interval width, LF and LW start to share similarities. However, for small intervals, resetting can be beneficial for LW also in the domain where the coefficient of variation is smaller than 1, which wasn't observed in case of LF.

[1] B. Żbik, and B. Dybiec, Phys. Rev. E 109, 044147 (2024).