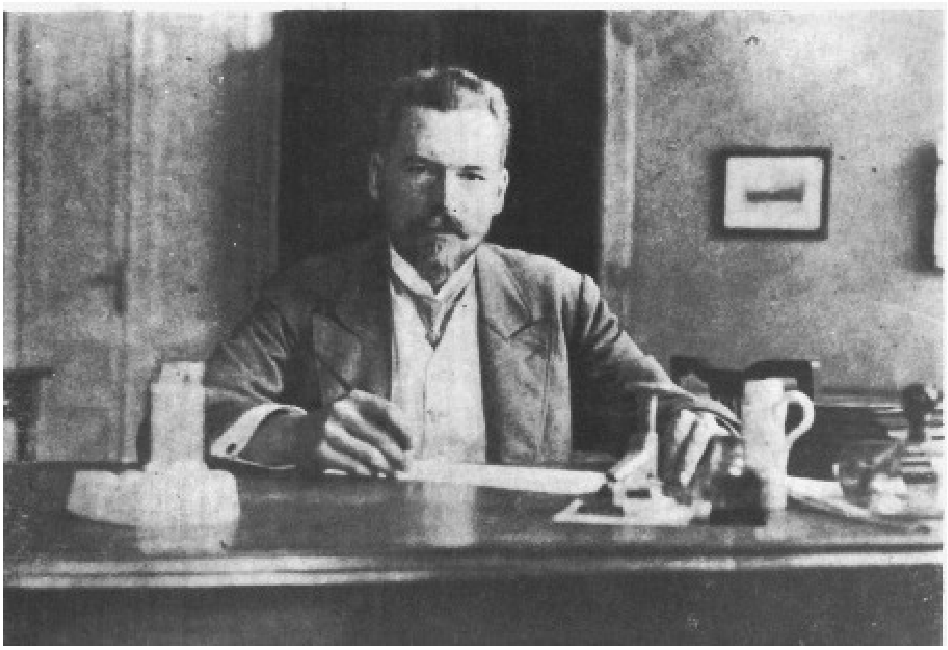
35th M. Smoluchowski Symposium on Statistical Physics



Report of Contributions

https://zakopane.if.uj.edu.pl/e/smoluchowski2022

Contribution ID: **2** Type: **Regular talk**

Statistical mechanics of adaptive neural networks: Explaining coexistence of avalanches and oscillations in resting human brain

Saturday, September 17, 2022 5:40 PM (25 minutes)

Neurons in the brain are wired into adaptive networks that exhibit a range of collective dynamics. Oscillations, for example, are paradigmatic synchronous patterns of neural activity with a defined temporal scale. Neuronal avalanches, in contrast, are scale-free cascades of neural activity, often considered as evidence of brain tuning to criticality. While models have been developed to account for oscillations or avalanches separately, they typically do not explain both phenomena, are too complex to analyze analytically, or intractable to infer from data rigorously. Here we propose a non-equilibrium feedback-driven Ising-like class of neural networks that simultaneously and quantitatively captures scale-free avalanches and scale-specific oscillations. In the most simple yet fully microscopic model version we can analytically compute the phase diagram and make direct contact with human brain resting-state activity recordings via tractable inference of the model's two essential parameters. The inferred model quantitatively captures the dynamics over a broad range of scales, from single sensor oscillations and collective behaviors of nearly-synchronous extreme events on multiple sensors, to neuronal avalanches unfolding over multiple sensors across multiple time bins. Importantly, the inferred parameters correlate with model-independent signatures of "closeness to criticality", indicating that the coexistence of scale-specific (neural oscillations) and scale-free (neuronal avalanches) dynamics in brain activity occurs close to a non-equilibrium critical point at the onset of self-sustained oscillations.

Primary authors: LOMBARDI, Fabrizio (Institute of Science and Technology Austria); Mr PEPIC, Selver (Institute of Science and Technology); Prof. SHRIKI, Oren (Ben Gurion University of the Negev); Prof. TKACIK, Gasper (Institute of Science and Technology Austria); Dr DE MARTINO, Daniele (Biofisika Institute (CSIC,UPV-EHU) and Ikerbasque Foundation)

Presenter: LOMBARDI, Fabrizio (Institute of Science and Technology Austria)

Session Classification: Saturday session

Contribution ID: **3** Type: **Regular talk**

Resolving a single-atom ”thermodynamic limit” in cavity QED: photon correlations and field distributions in the strong-coupling regime

Tuesday, September 20, 2022 4:20 PM (25 minutes)

We approach the strong-coupling “thermodynamic limit” in the open driven Jaynes-Cummings (JC) model. We do so by highlighting the role of quantum fluctuations against the predictions of mean-field theory in three distinct regimes of operation. We set the stage by demonstrating the persistence of photon blockade, predicted in [H. J. Carmichael, Phys. Rev. X 5, 031028 (2015)], as a manifestation of the inherently quantum and nonlinear JC spectrum revealed for vanishing photon loss. To assess the multiphoton resonances, we focus on the buildup and collapse of phase-space multimodality in the limit of weak drive where a perturbative treatment is possible. Correlation functions of the forwards and side-scattered photons provide an alternative perspective, uncovering conditional dynamics that are shaped by features unique to the ladder of JC eigenstates. We then proceed to the region of amplitude bistability for a drive amplitude of the same order of magnitude as the light-matter coupling strength. This finally brings us to the critical point of the well-known second-order quantum phase transition on resonance, where the quantum and semi-classical pictures are once more contrasted as we go through the collapse of the JC quasienergy spectrum.

Primary author: Dr MAVROGORDATOS, Themistoklis (ICFO - The Institute of Photonic Sciences)

Presenter: Dr MAVROGORDATOS, Themistoklis (ICFO - The Institute of Photonic Sciences)

Session Classification: Tuesday session

Contribution ID: **4** Type: **Poster**

Anomalous transport in driven periodic systems: distribution of the absolute negative mobility effect

Sunday, September 18, 2022 4:45 PM (3 minutes)

Absolute negative mobility is one of the most paradoxical forms of anomalous transport behaviour. At the first glance it contradicts the superposition principle and the second law of thermodynamics, however, its fascinating nature bridges nonlinearity and nonequlibrium state in which these fundamental rules are no longer valid. We consider a paradigmatic model of the nonlinear Brownian motion in a driven periodic system which exhibits the absolute negative mobility. So far research on this anomalous transport feature has been limited mostly to the single case studies due to the fact that this model possesses the complex multidimensional parameter space. In contrast, here we harvest GPU supercomputers to analyze the distribution of negative mobility in the parameter space. We consider nearly 10^9 parameter regimes to discuss how the emergence of negative mobility depends on the system parameters as well as provide the optimal ones for which it occurs most frequently.

Primary authors: WIŚNIEWSKI, Mateusz (University of Silesia in Katowice); Prof. SPIECHOWICZ, Jakub (University of Silesia in Katowice)

Presenter: WIŚNIEWSKI, Mateusz (University of Silesia in Katowice)

Session Classification: Poster session party

Contribution ID: **5** Type: **Regular talk**

RNA dynamics in the cytoplasm of mammalian cells

Monday, September 19, 2022 3:55 PM (25 minutes)

We study the motion of individual messenger RNA (mRNA) in the cytoplasm of HeLa cells using single-molecule tracking. The trajectories are analyzed in terms of the mean squared displacement and the power spectral density. We observe that the motion resembles an antipersistent random walk, which suggests fractional Brownian motion as a useful model. However, the trajectories alternate between different states due to cellular heterogeneities and interactions with specific partners. Interestingly, mRNA dynamics exhibit aging and ergodicity breaking. In order to shed light on the process, we compare the mRNA trajectories to that of semiconductor nanocrystals that were introduced into the cytoplasm. Statistical analyses of these trajectories also reveal sub-diffusion with antipersistent increments and substantial heterogeneities. Furthermore, particles randomly switch between different mobility states, which can be dissected using a hidden Markov model. Our data indicate that one of these states is rooted in the transient associations with the cytoskeleton-shaken endoplasmic reticulum network. We find that the nanocrystal motion serves as a good baseline for understanding the dynamics of biological molecules in the cell, but in the latter, specific interactions introduce additional complexities.

Primary authors: Mr ROESSLER, Ryan (Colorado State University); Dr WIGGAN, O'Neil (Colorado State University); Dr JANCZURA, Joanna (Wroclaw University of Science and Technology); Mr BALCEREK, Michal (Wroclaw University of Science and Technology); Dr BURNECKI, Krzysztof (Wroclaw University of Science and Technology); Prof. WEISS, Matthias (University of Bayreuth); Prof. STASEVICH, Tim (Colorado State University); KRAPF, Diego (Colorado State University)

Presenter: KRAPF, Diego (Colorado State University)

Session Classification: Monday session

Contribution ID: **6** Type: **Regular talk**

Quantum and classical contributions to entropy production in fermionic and bosonic systems

Sunday, September 18, 2022 4:20 PM (25 minutes)

As previously demonstrated, the entropy production – a standard measure of irreversibility of thermodynamic processes – is related to generation of correlations between degrees of freedom of the system and its environment [1]. A natural question appears whether such correlations are classical or quantum. This work deals with this problem by investigating noninteracting fermionic and bosonic systems. It is shown that for both classes of systems the entropy production is mostly related to the generation of quantum coherence in the eigenstate basis of the environment, namely, the Fock basis. This might suggest that the entropy production is mainly of a quantum origin. However, a more refined insight is provided by defining the classical correlations as a maximum amount of information accessible through measurements [2]. In fermionic systems measurements can be performed only in the Fock basis due to parity superselection rule forbidding the quantum superpositions of states with different particle parity [3]; therefore correlations are mostly quantum. For bosonic systems, however, a higher amount of information is provided by Gaussian measurements in the position-momentum phase space. While the position-momentum correlations are mostly quantum for low temperatures, they become purely classical in the high-temperature limit. This demonstrates a qualitative difference between fermionic and bosonic systems regarding the existence of a quantum-to-classical transition in microscopic description of the entropy production.

[1] New J. Phys. 12, 013013 (2010); Phys. Rev. Lett. 123, 200603 (2019)
[2] Phys. Rev. A 84, 042109 (2011)
[3] Phys. Rev. A 103, 032426 (2021)

Primary authors: Dr PTASZYŃSKI, Krzysztof (Institute of Molecular Physics, Polish Academy of Sciences); Prof. ESPOSITO, Massimiliano (Complex Systems and Statistical Mechanics, Department of Physics and Materials Science, University of Luxembourg)

Presenter: Dr PTASZYŃSKI, Krzysztof (Institute of Molecular Physics, Polish Academy of Sciences)

Session Classification: Sunday session

Contribution ID: **7** Type: **Regular talk**

Activity driven transport in extended systems

The transport properties of an extended system driven by active reservoirs is an issue of paramount importance, which remains virtually unexplored. Here we address this issue, for the first time, in the context of energy transport between two active reservoirs connected by a chain of harmonic oscillators. The couplings to the active reservoirs, which exert correlated stochastic forces on the boundary oscillators, lead to fascinating behavior of the energy current and kinetic temperature profile even for this linear system. We analytically show that the stationary active current (i) changes non-monotonically as the activity of the reservoirs are changed, leading to a negative differential conductivity (NDC), and (ii) exhibits an unexpected direction reversal at some finite value of the activity drive. The origin of this NDC is traced back to the Lorentzian frequency spectrum of the active reservoirs. We provide another physical insight to the NDC using nonequilibrium linear response formalism for the example of a dichotomous active force. We also show that despite an apparent similarity of the kinetic temperature profile to the thermally driven scenario, no effective thermal picture can be consistently built in general. However, such a picture emerges in the small activity limit, where many of the well-known results are recovered.

Primary authors: SANTRA, Ion (Raman Research Institute); Prof. BASU, Urna (S.N. Bose National Centre for Basic Sciences)

Presenter: SANTRA, Ion (Raman Research Institute)

Session Classification: Tuesday session

Contribution ID: **8** Type: **Regular talk**

Anomalous diffusion originated by two Markovian hopping-trap mechanisms

Wednesday, September 21, 2022 12:20 PM (25 minutes)

We show through intensive simulations that the paradigmatic features of anomalous diffusion are indeed the features of a (continuous-time) random walk driven by two different Markovian hopping-trap mechanisms. If $p \in (0, 1/2)$ and $1 - p$ are the probabilities of occurrence of each Markovian mechanism, then the anomalousness parameter $\beta \in (0, 1)$ results to be $\beta \boxtimes 1 - 1/\{1 + \log[(1 - p)/p]\}$. Ensemble and single-particle observables of this model have been studied and they match the main characteristics of anomalous diffusion as they are typically measured in living systems. In particular, the celebrated transition of the walker's distribution from exponential to stretched-exponential and finally to Gaussian distribution is displayed by including also the Brownian yet non-Gaussian interval.

The talk is based on: Vitali S., Paradisi P. and Pagnini G., J. Phys. A: Math. Theor. 55 (2022) 224012

Primary authors: PAGNINI, Gianni (BCAM - Basque Center for Applied Mathematics); Dr VITALI, Silvia (BCAM-Basque Center for Applied Mathematics); Dr PARADISI, Paolo (ISTI-CNR, Institute of Information Science and Technologies 'A. Faedo')

Presenter: PAGNINI, Gianni (BCAM - Basque Center for Applied Mathematics)

Session Classification: Wednesday session

Contribution ID: **9** Type: **Invited talk**

Linear response and fluctuiation-dissipation relations for stochastic processes under resetting

Saturday, September 17, 2022 3:00 PM (45 minutes)

We discuss a general situation of a response of a random process under stochastic resetting to an external force. The displacement process is considered to be a Markov one, and it starts anew at resetting events which follow a renewal process (complete resetting). When assuming that the displacement process shows linear response to a weak external force, we ask what kind of the response does the reset process show, and under what conditions usual fluctuation-dissipation relations (FDRs) or the generalized Einstein's relations (GERs) apply for this process. After discussing the general approach we turn to a specific example of a Brownian motion under resetting with arbitrary waiting time distribution between the resetting events for which many properties can be explicitly calculated. We show that if the distribution of waiting times of the resetting process possesses the second moment, the usual FDR applies for the response function of the coordinate, and if the second moment diverges but the first one stays finite, the static susceptibility diverges, but the GER still applies. In any of these situations, the fluctuation dissipation relations define the effective temperature of the system which is twice as high as the temperature of the medium in which the Brownian motion takes place.

Primary author: SOKOLOV, Igor (Humbold University at Berlin)

Presenter: SOKOLOV, Igor (Humbold University at Berlin)

Session Classification: Saturday session

Contribution ID: **10** Type: **Poster**

Random walks in correlated diffusivity landscapes

Sunday, September 18, 2022 5:15 PM (3 minutes)

The probability density function (PDF) of the displacement of particles moving in strongly disordered diffusivity landscapes shows an unusual way of convergence to a Gaussian under homogenization[1]. Namely, at finite times the PDF exhibits a sharp central peak, and the convergence to a Gaussian follows not by smoothing of the PDF but by narrowing of this central peak, which stays sharp even at long times. This particular feature is absent in all pre-averaged (mean field) approaches. In our poster we discuss this situation, and present the results of new numerical simulations of random walks on lattices with correlated waiting times on the sites. We show that the existence of the central peak is connected with strong correlations between the spatial and temporal aspects of walks on such landscapes, and that decoupling these correlations leads to a mean-field-like behavior without central peak. The correlations in waiting times along the trajectory of a walk alone (as taken into account in the diffusing-diffusivity type of models) are not able to reproduce the behavior. This understanding is important for building a mathematical model which could be able to describe the above mentioned features.

1. Adrian Pacheco-Pozo, Igor M Sokolov, Convergence to a Gaussian by narrowing of central peak in Brownian yet non-Gaussian diffusion in disordered environments, PRL 127 120601 (2021)

Primary author: PACHECO-POZO, Adrian (Humboldt Universität zu Berlin)

Co-author: SOKOLOV, Igor (Humbold University at Berlin)

Presenter: PACHECO-POZO, Adrian (Humboldt Universität zu Berlin)

Session Classification: Poster session party

Contribution ID: **11** Type: **Poster**

Fluctuations of work and heat in a driven entropic potential

Sunday, September 18, 2022 5:12 PM (3 minutes)

We consider the motion of an over-damped Brownian particle in two-dimensional bilobal confinement driven by a periodic field in the presence of a transverse bias force (G). The confinement results in an entropic bistable potential in a reduced dimension. We calculate the work done and absorbed heat over a period and their mean and relative variance fluctuations in entropy and energy-dominated regimes. This system exhibits the entropic stochastic resonance phenomena. The stochastic resonance phenomena can be described by the mean value of work done and absorbed heat over a period as function of noise strength and frequency input. It is found that the heat fluctuations over a single period are always greater than the work fluctuations. We also discuss the applicability of steady-state fluctuation theorems in this system.

Primary author: Mr ALI, Syed Yunus Ali (Indian Institute of Technology Tirupati)

Presenter: Mr ALI, Syed Yunus Ali (Indian Institute of Technology Tirupati)

Session Classification: Poster session party

Contribution ID: **12** Type: **Poster**

Colossal Brownian yet non-Gaussian diffusion in a periodic potential: impact of nonequilibrium noise amplitude statistics

Sunday, September 18, 2022 5:09 PM (3 minutes)

In [Phys. Rev. E 102, 042121 (2020)] the authors studied an overdamped dynamics of nonequilibrium noise driven Brownian particle dwelling in a spatially periodic potential and discovered a novel class of Brownian, yet non-Gaussian diffusion. The mean square displacement of the particle grows linearly with time and the probability density for the particle position is Gaussian, however, the corresponding distribution for the increments is non-Gaussian. The latter property induces the colossal enhancement of diffusion, significantly exceeding the well known effect of giant diffusion. Here we considerably extend the above predictions by investigating the influence of nonequilibrium noise amplitude statistics on the colossal Brownian, yet non-Gaussian diffusion. The tail of amplitude distribution crucially impacts both the magnitude of diffusion amplification as well as Gaussianity of the position and increments statistics. Our results carry profound consequences for diffusive behaviour in nonequilibrium settings such as living cells in which diffusion is a central transport mechanism.

Primary author: BIAŁAS, Karol (University of Silesia in Katowice)

Co-author: Prof. SPIECHOWICZ, Jakub (University of Silesia in Katowice)

Presenter: BIAŁAS, Karol (University of Silesia in Katowice)

Session Classification: Poster session party

Contribution ID: **13** Type: **Poster**

Single molecule characterization of protein-protein interactions between the heterogeneous plasma membrane and the cytoplasm of living cells

Sunday, September 18, 2022 5:06 PM (3 minutes)

Based on simultaneous three-color imaging of fluorescently labelled receptors, arrestins and clathrin coated pits, in living cells, we will analyze the dynamics and interaction patterns of membrane bound Adrenergic receptors with cytoplasmic β-arrestin 2 molecules as well as their recruitment to clathrin-coated pits structures (CCP) before internalization.
First, we demonstrate that arrestin molecules naturally undergo surface mediated diffusion alterning between bulk and membrane diffusion. Then, we analyze trajectories of individual receptors and membrane-bound arrestins by identifying over time whether molecules laterally diffuse on the membrane or are confined in some nano-domains by detecting transient trapping events [1]. Next, we study the colocalization of confined trajectories portions with clathrin-coated pits to determine whether confined portions are trapped in CCP or not. Subsequently, we proceed with the analysis of interactions between receptors and arrestins based on colocalization that allows us to quantify the association and dissociation rates. From the combination of information on confinement/trapping in CCP/Colocalization with a different protein we define states of receptor/arrestin over time from which we reconstruct the sequence of events before and after interactions of the molecules as well as the sequences of events leading to CCP recruitment.
Finally, we take advantage of our methodology to compare the effect of a change in biological conditions onto the dynamics and interaction kinetics of receptor/arrestin. This allows us to study the spatio-temporal changes related to receptor activation as well as different receptor affinity to arrestin. Also, we show how at a single-molecule level, one can correlate structural components of arrestin proteins to their role direct effect on receptor/arrestin kinetics and recruitment to CCP based on the analysis of multiple arrestin mutants. Our study [2] sheds new light on spatio-temporal character of receptor/arrestin interaction based on single molecules.

[1] Lanoiselée Y, Grimes J, Koszegi Z, Calebiro D. Detecting Transient Trapping from a Single Trajectory: A Structural Approach. Entropy. 2021; 23(8):1044. https://doi.org/10.3390/e23081044
[2] Grimes J, Koszegi Z, Lanoiselée Y, Miljus T, Mistry R, Stepniewski TM, Medel Lacruz B, Selent J, Hill SJ, Calebiro D. Single-molecule characterization of receptor – β-arrestin interactions. (In revision)

Primary authors: Dr LANOISELÉE, Yann (University of Birmingham); Mr GRIMES, Jak; Dr KOSZEGI, Zsombor (University of Birmingham); Prof. CALEBIRO, Davide (University of Birmingham)

Presenter: Dr LANOISELÉE, Yann (University of Birmingham)

Session Classification: Poster session party

Contribution ID: **14** Type: **Regular talk**

Temperature and friction fluctuations inside a harmonic potential

Tuesday, September 20, 2022 3:55 PM (25 minutes)

In this talk we present the study of the trapped motion of a molecule undergoing diffusivity fluctuations inside a harmonic potential. For the same diffusing-diffusivity process, we investigate two possible interpretations. Depending on whether diffusivity fluctuations are interpreted as temperature or friction fluctuations, we show that they display drastically different statistical properties inside the harmonic potential. We compute the characteristic function of the process under both types of interpretations and analyse their limit behavior. Based on the integral representations of the processes we compute the mean-squared displacement and the normalized excess kurtosis. In the long-time limit, we show for friction fluctuations that the probability density function (PDF) always converges to a Gaussian whereas in the case of temperature fluctuations the stationary PDF can display either Gaussian distribution or generalized Laplace (Bessel) distribution depending on the ratio between diffusivity and positional correlation times.

Temperature and friction fluctuations inside a harmonic potential
Yann Lanoiselée, Aleksander Stanislavsky, Davide Calebiro, Aleksander Weron (submitted)
https://arxiv.org/abs/2207.14068

Primary authors: Dr LANOISELÉE, Yann (University of Birmingham); Dr STANISLAVSKY, Aleksander (Institute of Radio Astronomy, Karkhiv); Prof. CALEBIRO, Davide (University of Birmingham); Prof. WERON, Aleksander (Faculty of Pure and Applied Mathematics, Hugo Steinhaus Center, Wroclaw)

Presenter: Dr LANOISELÉE, Yann (University of Birmingham)

Session Classification: Tuesday session

Contribution ID: **15** Type: **Poster**

Spectral analysis of the collective diffusion of Brownian particles confined to a spherical surface.

Sunday, September 18, 2022 5:03 PM (3 minutes)

A more fundamental understanding of non-equilibrium phenomena involving fluids confined to restricted geometries presents indeed a difficult challenge. Here we explore a novel approach to describe the collective diffusion of Brownian particles confined to a spherical surface by adapting the dynamic density functional theory (DDFT) to this geometry [1]. The ensuing diffusion equation is then transformed into a system of coupled ordinary differential equations by implementing spherical harmonics expansions of the relevant functions. This study is complemented with Brownian dynamics (BD) simulations performed with an innovative extension of the Ermak–McCammon algorithm, while employing conditional ensemble averages over initial non-equilibrium states. In both cases the relaxations processes are analyzed through the decay modes obtained from the spectral method. The simple DDFT approach considered here provides a fairly good description of the BD results. In particular, the theoretical predictions for the initial progression rates of the local density modes turn out to be almost exact, and we found that this can be explained in terms of the eigenvalues and eigenvectors corresponding to an initial renormalized potential. As an illustration, the model system has been tailored to the experimental conditions of Pickering emulsions stabilized by functionalized gold nanoparticles.

[1] A. Montañez-Rodríguez, C. Quintana, and P. González-Mozuelos, Spectral analysis of the collective diffusion of Brownian particles confined to a spherical surface, Physica A: Statistical Mechanics and its Applications 574, 126012 (2021).

Primary authors: MONTAÑEZ-RODRÍGUEZ, A.; QUINTANA, C.; GONZÁLEZ-MOZUELOS, P.

Presenter: MONTAÑEZ-RODRÍGUEZ, A.

Session Classification: Poster session party

Contribution ID: **16** Type: **Regular talk**

Solitons in driven overdamped Brownian motion

Tuesday, September 20, 2022 9:55 AM (25 minutes)

In systems with inertia, solitons are waves whose dispersion is suppressed by nonlinear effects. We demonstrate that solitons can occur also in the absence of inertia in overdamped dynamics of Brownian hard spheres driven through periodic potentials at high density. In such systems, the dispersion of density waves is suppressed due to the fact that particles keep together in clusters and external forces are not able to separate them. The motion of clusters can induce particle currents even in the zero-noise limit, where transport of single particles over potential barriers is not possible. The structure of the particle current suggests that solitons dominate the particle current also at high noise. The predicted effects can occur in a broad class of periodic systems.

1. Solitons in overdamped Brownian dynamics,
   Alexander P. Antonov, Artem Ryabov, and Philipp Maass,
   to appear in Phys. Rev. Lett. (2022)
   arXiv:2204.14181, DOI: 10.48550/arXiv.2204.14181
2. Collective excitations in jammed states: ultrafast defect propagation and finite-size scaling,
   Alexander P. Antonov, David Voráč, Artem Ryabov, and Philipp Maass,
   arXiv:2203.06372 (2022), DOI: 10.48550/arXiv.2203.06372

Primary authors: RYABOV, Artem (Charles University); ANTONOV, Alexander (Universität Osnabrück); MAASS, Philipp (Universität Osnabrück)

Presenter: RYABOV, Artem (Charles University)

Session Classification: Tuesday session

Contribution ID: **17** Type: **Poster**

Microscopically reversible active dynamics at the nanoscale

Sunday, September 18, 2022 5:00 PM (3 minutes)

Catalytically active nanoparticles are envisioned as principal components for artificial nanomotors. However, theory and experiments report conflicting findings regarding their dynamics. The lack of consensus is mostly caused by a limited understanding of self-propulsion mechanisms at the nanoscale. Here, we focus on a fundamental symmetry of kinetics of catalytic reactions powering the self-propelled motion: we shall assume the microscopic reversibility of this kinetics and demonstrate significant and qualitative effects stemming from this assumption that arise if nanoparticles are subjected to an action of external forces. Since microscopic reversibility is a generic property of several chemical reactions, the results can provide new insights into the dynamics of a broad class of nanoparticles.

[1] A. Ryabov and M. Tasinkevych, Soft Matter 18, 3234-3240 (2022), DOI: 10.1039/D2SM00054G

[2] A. Ryabov and M. Tasinkevych, arXiv:2206.00616 (2022), DOI: 10.48550/arXiv.2206.00616

Primary authors: RYABOV, Artem (Charles University); TASINKEVYCH, Mykola (Nottingham Trent University)

Presenter: RYABOV, Artem (Charles University)

Session Classification: Poster session party

Contribution ID: **18** Type: **Regular talk**

Learning from onion to balance between order and chaos

Saturday, September 17, 2022 3:55 PM (25 minutes)

Recent progress in fabrication methods draws attention to lattice materials. Thanks to their structure lattice materials frequently offer superior performance compared to bulk materials. However, most of them suffer from shear bands. These strain localizations, diagonal to the load direction, are the main mode of failure for lattice materials. Sear bands are due to a very organized periodic structure of lattice materials. Introducing randomness to the lattice structure helps to eliminate shear bands but introduces force chains - an unwelcome feature typical for materials with a random structure, such as sand or paper. In this presentation, we show a bio-inspired material that is neither completely random nor periodic. Such engineered material should be immune to problems of both periodic and chaotic materials. This honeycomb material has a structure inspired by the epidermis tissue of an onion. This tissue is characterized by large fluctuations in cell sizes. There is a threefold difference in the length of the cells. However, the cells are not completely randomly distributed. There is a certain correlation between the cells so as to avoid stiff connections that lead to unwanted force chains. We aim to build a "tissue generator " which will create a cellular structure mimicking the onion epidermis in every aspect. In order to select the algorithm that mimics the onion tissue most faithfully, we test several algorithms that lead to onion-like cell structure using statistical methods. The structure that passes the tests is 3D printed and tested mechanically to determine its failure modes. It is modeled using the finite element method to investigate the stress distribution.

Primary author: KRZEMIEN, Leszek (Instytut Katalizy i Fizykochemii Powierzchni im. Jerzego Habera Polskiej Akademii Nauk)

Co-author: BARBASZ, Jakub (Instytut Katalizy i Fizyochemii Powierzchni im. Jerzego Habera PAN)

Presenter: KRZEMIEN, Leszek (Instytut Katalizy i Fizykochemii Powierzchni im. Jerzego Habera Polskiej Akademii Nauk)

Session Classification: Saturday session

Contribution ID: **19** Type: **Poster**

Essential requisites for best performance of Geometric Brownian Information Engine.

Sunday, September 18, 2022 4:57 PM (3 minutes)

We investigate a Geometric Brownian Information Engine (GBIE) in the presence of an error-free feedback controller that transforms the information gathered on the state of particles entrapped in mono-lobal geometric detention into extractable work[1,2]. We determine the benchmarks for utilizing the available information in an output work and the optimum operating requisites for best performance. Apart from a reference measurement distance xm and feedback site xf , upshots of the information engine also depend on the transverse constant bias force (G)[3]. G tunes the entropic contribution in the effective potential and the standard deviation (σ) of the equilibrium marginal probability distribution. We find that the upper bound of the achievable work shows a crossover from (5/3-2ln2)kBT to 1/2kBT when the system changes from entropy to an energy-dominated one. The higher loss of information during the relaxation process accredits the lower value of work in entropic instances of GBIE. We recognize that the work extraction reaches a global maximum when xf=2xm with xm ⊠ 0.6σ, irrespective of the extent of the entropic limitation. Also, we explore the effect of entropic control on the unidirectional passage of the particle and efficacy of the GBIE[4].

1. R. Zwanzig, J. Phys. Chem. 96,3926 (1992).
2. T. Sagawa and M. Ueda, Phys. Rev. Lett. 104, 090602 (2010).
3. T. Sagawa, and M. Ueda, Phys. Rev. E„ 85, 021104(2012).
4. R. Rafeek, S. Y. Ali, and D. Mondal, Communicated (2022).

Primary authors: Ms RAFEEK, Rafna (Department of Chemistry and Center for Molecular and Optical Sciences & Technologies, Indian Institute of Technology Tirupati, Yerpedu 517619, Andhra Pradesh,India); Mr ALI, Syed Yunus (Department of Chemistry and Center for Molecular and Optical Sciences & Technologies, Indian Institute of Technology Tirupati, Yerpedu 517619, Andhra Pradesh,India); Dr MONDAL, Debsish (Department of Chemistry and Center for Molecular and Optical Sciences & Technologies, Indian Institute of Technology Tirupati, Yerpedu 517619, Andhra Pradesh,India)

Presenter: Ms RAFEEK, Rafna (Department of Chemistry and Center for Molecular and Optical Sciences & Technologies, Indian Institute of Technology Tirupati, Yerpedu 517619, Andhra Pradesh,India)

Session Classification: Poster session party

Contribution ID: **20** Type: **Poster**

First or second? An attempt to determine the order of a phase transition with machine learning methods.

Sunday, September 18, 2022 4:54 PM (3 minutes)

The determination of the order of a phase transition can be quite a challenging task. In the thermodynamic limit the situation is clear: in the case of a first–order phase transition we observe discontinuity in the free energy at the critical point leading to the release of a latent heat. This phenomenon is not observable in the case of a continuous phase transition. Therefore, the results obtained with Monte Carlo computations, which simulate only the finite–size systems do not always provide an answer whether transition is of first or second–order. We attempt to overcome this issue by a careful analysis of the output obtained from the application of the learning by confusion scheme to the Potts, Blume–Capel and Falicov–Kimball models. We discover that in some cases the establishment of the order of a phase transition is plausible, but the results obtained in the case of a discontinuous phase transition strictly depend on the number of degrees of freedom and their character (quantum, classical).

Primary authors: Mrs RICHTER-LASKOWSKA, Monika (Institute of Medical Technology and Equipment); Dr KURPAS, Marcin; Prof. MAŚKA, Maciej

Presenter: Mrs RICHTER-LASKOWSKA, Monika (Institute of Medical Technology and Equipment)

Session Classification: Poster session party

Contribution ID: **21** Type: **Regular talk**

Geometric Brownian Information Engine

Monday, September 19, 2022 9:55 AM (25 minutes)

We design a geometric Brownian information engine by considering over-damped Brownian particles inside a two-dimensional monolobal confinement with irregular width along the transport direction. Under such detention, particles experience an effective entropic potential which has a logarithmic form. We employ a feedback control protocol as an outcome of error-free position measurement [1-2]. The protocol comprises three stages: measurement, feedback and relaxation. We reposition the center of the confinement to the measurement distance instantaneously when the position of the trapped particle crosses for the first time. Then, the particle is allowed to thermal relaxation. We calculate the extractable work, total information and unavailable information associated with the feedback control using this equilibrium probability distribution function. We find the exact analytical value of the upper bound of extractable work as [2]. We introduce a constant force G downwards to the transverse coordinate (y). A change in G alters the effective potential of the system and tunes the relative dominance of entropic and energetic contributions in it. The upper bound of the achievable work shows a cross-over from to when the system changes from an entropy dominated regime to energy dominated one [3]. Compared to an energetic analogue, the loss of information during the relaxation process is higher in the entropy-dominated region, which accredits the less value in achievable work. We also determine the benchmarks for utilizing the available information in an output work and the optimum operating requisites for best performance [4].

[1] T. Sagawa and M. Ueda, Phys. Rev. Lett. 104, 090602 (2010).
[2] Y. Ashida, K. Funo, Y. Murashita, and M. Ueda, Phys. Rev. E, 90, 052125 (2014).
[3] S. Y. Ali, R. Rafeek and D. Mondal, J. Chem. Phys, 156, 014902 (2022).
[4] R. Rafeek, S. Y. Ali, and D. Mondal, Communicated (2022).

Primary author: Dr MONDAL, Debasish (Indian Institute of Technology Tirupati, Yerpedu 517619, Andhra Pradesh, India)

Presenter: Dr MONDAL, Debasish (Indian Institute of Technology Tirupati, Yerpedu 517619, Andhra Pradesh, India)

Session Classification: Monday session

Contribution ID: **22** Type: **Regular talk**

A human-size realisation of the Feynman–Smoluchowski ratchet-and-pawl thought experiment

Monday, September 19, 2022 10:20 AM (25 minutes)

We take inspiration from Feynman–Smoluchowski ratchet-and-pawl thought experiment to build experimentally a Maxwell's demon at human-size.
We use a centimeter blade shafted to a CC-motor. Then, the blade is immersed in a granular gas made of hundreds of millimeter steal beads. The gas stands for an out-of-equilibrium heat bath, and the blade stands for a 1D Brownian particle whose speed is measured by the voltage at the motor connectors.
In Feynman–Smoluchowski thought experiment, the blade is free to rotate in one direction but the ratchet-and-pawl prevent rotation in the other direction.
To that end, in our experiment, we plug a diode and a load on the CC-motor in order to exert back-action depending on the blade speed. This demon introduces an asymmetry in the Brownian motion of the blade that thus experiences a neat motion in one well-defined direction
We analyze both dynamical and statistical properties of the particle motion. and even measure a thermodynamical quantities such as work, heat or efficiency.

Primary author: Mr LAGOIN, Marc (Laboratoire de Physique ENS de Lyon)

Presenter: Mr LAGOIN, Marc (Laboratoire de Physique ENS de Lyon)

Session Classification: Monday session

Contribution ID: **23** Type: **Poster**

The investigation of BK ion channels activity using the method of Empirical Mode Decomposition

Sunday, September 18, 2022 4:51 PM (3 minutes)

The ion channels are characterized by a high degree of complexity, largely sensitive to the measurement conditions. The complex dynamics of the processes taking place in biological membranes is nontrivial and difficult to describe by the standard techniques dedicated to signal analysis. It is still unclear what specific mechanism leads to pink noise, which is an averaged effect of ion channel dynamics [2].
In this work the ionic conductivity signals of BK channels are decomposed into a finite number of empirical components, using a procedure called Empirical Mode Decomposition (EMD) pioneered by N. E. Huang et al. [1]. To fully understand the principles underlying these complex microbiological systems, the received frequency components were carefully analyzed through the methods dedicated to nonlinear and non-stationary signals: multifractal techniques and information entropy. These nonlinear features of the ion channels system activity strongly depend on the sampling rate at patch-clamp recording.
The modes extraction technique in conjunction with the implementation of the complexity measures allows for a better understanding of the structure of the time series and the process hidden behind the data including impact of individual components with different frequency characteristics on the entire signal.

REFERENCES

[1] N. E. Huang et.al,The empirical mode decomposition and hilbert spectrum for nonlinear and nonstationary time series analysis. Proc. Roy. Soc. London A, 454, 903–995, 1998.
[2] Machura, L., Wawrzkiewicz-Jałowiecka, A., Bednarczyk, P., & Trybek, P. (2022). Linking the sampling frequency with multiscale entropy to classify mitoBK patch-clamp data. Biomedical Signal Processing and Control, 76, 103680.

Primary authors: Dr TRYBEK, Paulina (University of Silesia in Katowice, Faculty of Science and Technology, Chorzów, 41-500, Poland); MACHURA, Lukasz (University of Silesia in Katowice, Faculty of Science and Technology, Chorzów, 41-500, Poland); WAWRZKIEWICZ-JALOWIECKA, Agata (Silesian University of Technology, Faculty of Chemistry); Dr BEDNARCZYK, Piotr (Department of Physics and Biophysics, Institute of Biology, Warsaw University of Life Sciences—SGGW)

Presenter: Dr TRYBEK, Paulina (University of Silesia in Katowice, Faculty of Science and Technology, Chorzów, 41-500, Poland)

Session Classification: Poster session party

Contribution ID: **24** Type: **Regular talk**

Natural time scales embedded in the mitoBK ion current dynamics

Wednesday, September 21, 2022 10:40 AM (25 minutes)

We address the two-fold applicability of the power spectrum density of the large-conductance voltage- and Ca2+ -activated potassium channels of the inner mitochondrial membrane (mitoBK). First, we will address the estimation of the optimal sampling frequency for the fibroblast's mitoBK patch-clamp data analysis [1], employing the process with doubly harmonic diminution, known to produce pink noise [2]. Next, we will discuss the ion current's empirical modes [3] in detail. We will show that the consecutive mode's power spectra show known 1/f characteristics. The brief correspondence of the instantaneous frequencies to the actual time scales will also be presented.

[1] L. Machura, A. Wawrzkiewicz-Jałowiecka, P. Bednarczyk, and P. Trybek, Linking the Sampling Frequency with Multiscale Entropy to classify mitoBK patch-clamp data, Biomed. Signal. Process. Control 76, 103680 (2022).
[2] P.M. Riechers, J.P. Crutchfield, Fraudulent white noise: Flat power spectra belie arbitrarily complex processes, Phys. Rev. Res. 3 013170 (2021).
[3] N.E. Huang et al., The empirical mode decomposition and the Hilbert spectrum for nonlinear and non-stationary time series analysis, Proc. R. Soc. Lond. A 454.1971 (1998).

Primary authors: MACHURA, Lukasz (University of Silesia); Dr TRYBEK, Paulina (University of Silesia in Katowice, Faculty of Science and Technology, Chorzów, 41-500, Poland); WAWRZKIEWICZ--JALOWIECKA, Agata (Silesian University of Technology, Faculty of Chemistry)

Presenter: MACHURA, Lukasz (University of Silesia)

Session Classification: Wednesday session

Contribution ID: **25** Type: **Regular talk**

Stability of gene expression patterns in developmental systems with dynamic morphogen sources

Saturday, September 17, 2022 4:20 PM (25 minutes)

In developmental systems cells determine their fate by decoding chemical signals, called morphogens. This results in the emergence of gene expression patterns. I will address the problem of gene expression patterns stability in the systems where two interacting and diffusible gene expression products control the size of their own source regions. Such systems are encountered in e.g. spinal cord development, limb formation and many others. The reaction-diffusion equation with threshold-activated production term is employed as a generic model for this problem. It is found that its dynamics is governed by the conservation law, which leads to a range of analytical results. In particular, phase transition is observed, between the phase of indeterminate patterning, where the region of mixed gene expression is ever growing, and the phase of travelling gene expression patterns, where two expression domains form a well-defined contact zone. A sub-class of genuinely stationary patterns is then identified, alongside the exact conditions ensuring this stability. These results allow me to classify all one- and two-gene regulatory motifs by their ability to produce stable patterns.

Primary author: MAJKA, Maciej (Jagiellonian University)

Presenter: MAJKA, Maciej (Jagiellonian University)

Session Classification: Saturday session

Contribution ID: **26** Type: **Poster**

Effect of drift on the motion of particles diffusing through a hybrid membrane

Sunday, September 18, 2022 4:48 PM (3 minutes)

The investigation of the influence of drift on the behavior of diffusing particles through a polymeric membrane filled with inorganic powder is considered. In this case, we use sodium alginate as a polymer matrix filled with iron oxide nanoparticles. Such membranes can be considered as a mixture of organic and inorganic phases. The first set of analyses examined the impact of drift on particles diffusing through real hybrid membranes. The second part focus on random walk simulations on artificial membrane structures. We investigate how the action of drift changes the properties of the diffusing particles through the hybrid membranes. We test the effect of two parameters such as the distribution of filling in the membrane and the value of drift on the nature of diffusion. It seems that the interaction between drift, diffusion, and the membrane structure affects the occurrence of the superdiffusive and subdiffusive character of particle motion. An important point is that the steady drift supports subdiffusive motion as it increases the chances of particle trapping. Furthermore, there exists an optimal value of drift, for which the transport through a membrane speeds up and does not cause trapping.

[1] G. Dudek, M. Krasowska, R. Turczyn, M. Gnus, A. Strzelewicz, Sep. Purif. Technol. 182 101–109 (2017).
[2] M. Krasowska, A. Strzelewicz, G. Dudek, M. Cieśla, Phys. Rev. E 95, 012155 (2017).
[3] A. Strzelewicz, M. Krasowska, G. Dudek, M. Cieśla, Chem. Phys. 531, 110662 (2020).
[4] A. Strzelewicz, M. Krasowska, G. Dudek, M. Cieśla, J. Mat. Sci. 57, 11491–11504 (2022).

Primary authors: KRASOWSKA, Monika (Silesian University of Technology); STRZELEWICZ, Anna (Silesian University of Technology); DUDEK, Gabriela (Silesian University of Technology); CIESLA, Michal (M. Smoluchowski Institute of Physics, Jagiellonian University, Kraków, Poland)

Presenter: CIESLA, Michal (M. Smoluchowski Institute of Physics, Jagiellonian University, Kraków, Poland)

Session Classification: Poster session party

Contribution ID: **27** Type: **Invited talk**

Finite-time dynamical phase transitions in non-equilibrium relaxation

Tuesday, September 20, 2022 3:00 PM (45 minutes)

Thermal relaxation is a fundamental process in statistical mechanics, with numerous applications in Nature and industry. Nonetheless, the kinetics of relaxation is well understood only close to equilibrium. Far-from-equilibrium relaxation, by contrast, is a genuine non-equilibrium problem that offers fascinating open questions, and a variety of unexpected phenomena.

In my talk, I will discuss a particular class of such phenomenona, namely finite-time dynamical phase transitions. These transitions occur during thermal relaxation after an instantaneous quench of the free energy landscape. They manifest themselves as finite-time cusp singularities in the probability distributions of thermodynamic observables. The transitions are due to sudden switches in the dynamics, and they are characterised by dynamical order parameters.

To classify these transitions, I will introduce a dynamical Landau theory that applies to a range of systems with scalar, parity-invariant order parameters. Close to criticality, the theory reveals an exact mapping between dynamical and equilibrium phase transitions, and implies critical exponents of mean-field type. Beyond the mean-field treatment, interactions between nearby saddle points may lead to critical, spatiotemporal fluctuations of the order parameter, and thus give rise to novel, dynamical critical phenomena.

Primary authors: Dr MEIBOHM, Jan (King's College London); Prof. ESPOSITO, Massimiliano (Complex Systems and Statistical Mechanics, Department of Physics and Materials Science, University of Luxembourg)

Presenter: Dr MEIBOHM, Jan (King's College London)

Session Classification: Tuesday session

Contribution ID: **28** Type: **Invited talk**

To thermalize or not to thermalize, that is the question

Sunday, September 18, 2022 3:00 PM (45 minutes)

In the first part of my lecture, I will discuss thermalization, ergodicity, and lack of them in classical systems. I will focus on paradigmatic example of spin glasses, and normal and anomalous diffusion processes. I will turn then to quantum closed systems, which, when perturbed or quenched, tend to "thermalize" in an ergodic way: the reduced density matrix of a block of the system is well approximated by the Gibbs-Boltzmann canonical ensemble, at least for averages of local observables and their-not-too-high-moments. There are several exceptions from this situation: i) Systems with multiple constants of motion are described by generalized Gibbs-Boltzmann ensembles; ii) Many-body localization (MBL) occurs in certain disordered systems; iii) MBL may occur also in non-disordered systems; iv) Local conservation laws, like the Gauss law, may prevent thermalization, for instance in Lattice Gauge Theory (LGT) models; v) Systems may exhibit quantum many-body scars, i.e. low entropy states that cause "weak" ergodicity breaking; vi) The latter occur frequently in confined LGT, but also in deconfined ones.

Primary author: LEWENSTEIN, Maciej (ICFO)

Presenter: LEWENSTEIN, Maciej (ICFO)

Session Classification: Sunday session

Contribution ID: **29** Type: **Invited talk**

Fractional Brownian motion with random Hurst exponent

Monday, September 19, 2022 3:00 PM (45 minutes)

Fractional Brownian motion, a Gaussian non-Markovian self-similar process with stationary long-correlated increments, has been identified to give rise to the anomalous diffusion behavior in a great variety of physical systems. The correlation and diffusion properties of this random motion are fully characterized by its index of self-similarity, or the Hurst exponent.
However, recent single particle tracking experiments in biological cells revealed highly complicated anomalous diffusion phenomena that cannot be attributed to a class of self-similar random processes. Inspired by these observations, we here study the process which preserves the properties of fractional Brownian motion at a single trajectory level, however, the Hurst index randomly changes from trajectory to trajectory. We provide a general mathematical framework for analytical, numerical and statistical analysis of fractional Brownian motion with random Hurst exponent. The explicit formulas for probability density function, mean square displacement and autocovariance function of the increments are presented for three generic distributions of the Hurst exponent, namely two-point, uniform and beta distributions. The important features of the process studied here are accelerating diffusion and persistence transition which we demonstrate analytically and numerically.

Primary author: Prof. WYŁOMANSKA, Agnieszka (Faculty of Pure and Applied Mathematics, Wroclaw University of Science and Technology)

Presenter: Prof. WYŁOMANSKA, Agnieszka (Faculty of Pure and Applied Mathematics, Wroclaw University of Science and Technology)

Session Classification: Monday session

Contribution ID: **30** Type: **Regular talk**

The versatile role of plastic crystals in light harvesting

Tuesday, September 20, 2022 12:35 PM (25 minutes)

One route towards capturing solar energy with great efficiency is to fundamentally investigate the way nature is capable of performing the different stages in photo-synthesis. Chlorosomes - large antennae complexes found in Green Sulfur Bacteria - are unique in capturing and transporting photon energy with near 100% quantum efficiency to the reaction centre where electrons and holes are separated for downstream usage. An interesting feature is that these huge antennae are able to perform an important biological function in the absence of regulatory proteins. Being composed of pigments only, chlorosomes offer a possibility for studying how light harvesting is encoded in the plastic-crystalline phase behavior and particularly in its dynamic disorder, and why the coupling between electronic, atomistic and molecular degrees of freedom gives rise to such great efficiency. Earlier, we performed systematic large-scale molecular dynamics (MD) simulations of chlorosomes in order to resolve the unknown pigment packing and the dynamic disorder within it. Next, we coupled this structure to a Frenkel Hamiltonian for calculating the exciton evolution and study the role of dynamic disorder in fast excitation energy transfer (EET), a mechanism that remains unresolved up to date. We found that the dynamic disorder, as encoded in a varying Frenkel Hamiltonian, has the effect of localising coherent domains, but that it at the same time accelerates transport of excitonic energy over the assembly structure via an enhanced mixing of overlapping eigenstates of very similar energy. In this presentation, we provide the details of this intriguing mechanism.

Primary author: SEVINK, Agur (Leiden University)

Co-authors: Dr LI, Xinmeng (Leiden University); Dr BUDA, Francesco (Leiden University); Prof. DE GROOT, Huub (Leiden University)

Presenter: SEVINK, Agur (Leiden University)

Session Classification: Tuesday session

Contribution ID: **31** Type: **Regular talk**

Anderson Localization of Composite Particles

Monday, September 19, 2022 12:10 PM (25 minutes)

We investigate the effect of coupling between translational and internal degrees of freedom of composite quantum particles on their localization in a random potential. We show that entanglement between the two degrees of freedom weakens localization due to the upper bound imposed on the inverse participation ratio by purity of a quantum state. We perform numerical calculations for a two-particle system bound by a harmonic force in a 1D disordered lattice and a rigid rotor in a 2D disordered lattice. We illustrate that the coupling has a dramatic effect on localization properties, even with a small number of internal states participating in quantum dynamics.

Phys. Rev. Lett. 127, 160602 (2021)

Primary authors: SUZUKI, Fumika (ISTA (Institute of Science and Technology Austria)); Prof. LEMESHKO, Mikhail (ISTA); Dr ZUREK, Wojciech (Los Alamos National Lab); Prof. KREMS, Roman (University of British Columbia)

Presenter: SUZUKI, Fumika (ISTA (Institute of Science and Technology Austria))

Session Classification: Monday session

Contribution ID: **32** Type: **Invited talk**

Finding low energy states of low-dimensional spin-glasses via approximate tensor network contractions.

Monday, September 19, 2022 11:15 AM (45 minutes)

I'll present a deterministic classical algorithm to efficiently sample high-quality solutions of certain spin-glass systems that encode hard optimization problems. It employes tensor networks to represent the Gibbs distribution of all possible configurations. Using approximate tensor-network contractions, we can efficiently map the low-energy spectrum of some quasi-two-dimensional Hamiltonians. Exploiting the local nature of the problems allows computing spin-glass droplets geometries, which provides a new form of compression of the low-energy spectrum. This naturally encompasses sampling, which otherwise, for exact contraction, is $\#P$ hard in general.

I'll discuss the performance of that approach in the context of existing and upcoming quantum annealing devices. I'll also show that inhomogeneous quantum annealing that employs information about the droplets may allow one to reach higher diversity of solutions than the standard homogeneous quantum annealing schedules.

Based on:

[1] M. M. Rams, M. Mohseni, D. Eppens, K. Jałowiecki, B. Gardas, Phys. Rev. E 104, 025308 (2021).
[2] M. Mohseni, M. M. Rams, et. al., arXiv:2110.10560
[3] A. Dziubyna, T. Śmierzchalski, B. Gardas, M. M. Rams, et. al., in prep.

Primary author: RAMS, Marek (Jagiellonian University in Kraków)

Presenter: RAMS, Marek (Jagiellonian University in Kraków)

Session Classification: Monday session

Contribution ID: **33** Type: **Invited talk**

Dynamics, fractal geometry and the exponents of the Kardar-Parisi-Zhang equation

Wednesday, September 21, 2022 9:55 AM (45 minutes)

The KPZ equation[1] is connected to a large number of processes, such as atomic deposition, evolution of bacterial colonies, the direct polymer model, the weakly asymmetric simple exclusion process, the totally asymmetric exclusion process, direct d-mer diffusion, fire propagation, turbulent liquid-crystal, spin dynamics, polymer deposition in semiconductors, and etching [2]. We present a short review of the field, some modern problems and perspectives. We discuss as well how a new interpretation of the fluctuation-dissipation theorem[3] allows us to give a solution for the KPZ exponents[4].

References

[1] M. Kardar, G. Parisi, and Y. C. Zhang, Phys. Rev. Lett. {\bf 56}, 9, 889 (1986).

[2] B. A. Mello, A. S. Chaves, and F. A. Oliveira, Phys. Rev. E \textbf{63}, 041113 (2001).
— E. A. Rodrigues, B. A. Mello, and F. A. Oliveira, J. Phys. A {\bf 48}, 035001 (2015).
— W. R. Gomes, A. L. A. Penna and F. A. Oliveira, Phys. Rev. E \textbf{100} 02101 (2019)

[3] M. S. Gomes-Filho, and F. A. Oliveira, EPL \textbf{133} 10001 (2021) — P. R. H. dos Anjos, W. S. Alves, M. S. Gomes-Filho, D. L. Azevedo and F. A. Oliveira, Frontiers in Physics 9 (https://doi.org/10.3389/fphy.2021.741590), 741590 (2021).

[4] M. S. Gomes-Filho, A. L. A. Penna and F. A. Oliveira, Results in Physics 26, \textbf{26} 104435 (2021).

Primary author: Prof. OLIVEIRA, Fernando (University of Brasilia)

Presenter: Prof. OLIVEIRA, Fernando (University of Brasilia)

Session Classification: Wednesday session

Contribution ID: **34** Type: **Regular talk**

On the scaling properties of spontaneous cell motility

Monday, September 19, 2022 4:20 PM (25 minutes)

Motility is one of the most salient aspects of cellular behavior. From the functional point of view, it is essential for many tasks cells perform, from forming tissues and organs during development to deploying the immune response during an infection. In addition, cell movements are usually easy to record, therefore allowing to perform quantitative studies of cell behavior.
Despite the advances in imaging and cell culture techniques of the last decades, there is still no agreement on the general laws that describe spontaneous cell movement. Moreover, the lack of a mechanistic model linking the activity of intracellular signaling cascades with spontaneous cell motility hinders our capacity to understand how cells integrate internal states and external cues into behavioral outputs.
Here we propose that cell behavior is the result of critical dynamics. To demonstrate this, we are required to show at least three types of evidence: i) scale-freeness and long-range correlations in the activity of intracellular signaling networks, ii) scaling behavior in spontaneous cell motility, and iii) collective phenomena emerging in the motility of groups of cells.
We will provide evidence from experiments and simulations to support this hypothesis, focusing on the scaling behavior of cells' spontaneous motility in different cell types and conditions. Furthermore, our results provide a framework for proposing new experiments and interpreting seemingly contradictory results from the literature.

Primary author: ZAMPONI, Nahuel (Weill Cornell Medicine)

Presenter: ZAMPONI, Nahuel (Weill Cornell Medicine)

Session Classification: Monday session

Contribution ID: **35** Type: **Invited talk**

New developments in relativistic dissipative hydrodynamics

Tuesday, September 20, 2022 9:00 AM (45 minutes)

Several recent developments in relativistic hydrodynamics are discussed with the emphasis on extensions aiming at description of highly off equilibrium systems (anisotropic hydrodynamics) and inclusion of spin polarization phenomena (spin hydrodynamics).

Primary author: FLORKOWSKI, Wojciech (Jagiellonian University)

Presenter: FLORKOWSKI, Wojciech (Jagiellonian University)

Session Classification: Tuesday session

Contribution ID: **37** Type: **Invited talk**

Collective dynamical regimes and synchronization transitions in spontaneous brain activity

Wednesday, September 21, 2022 11:35 AM (45 minutes)

The cerebral cortex exhibits spontaneous activity even in the absence of any task or external stimuli. A salient aspect of this resting-state dynamics, as revealed by in vivo and in vitro measurements, is that it exhibits several patterns, including collective oscillations, emerging out of neural synchronization, as well as highly-heterogeneous outbursts of activity interspersed by periods of quiescence, called "neuronal avalanches".
It has been conjectured that such a state is best described as a critical dynamical process—whose nature is still not fully understood—where scale-free avalanches of activity emerge at the edge of a phase transition.
In particular, some works suggest that this is most likely a synchronization transition, separating synchronous from asynchronous phases.
By investigating a simplified model of coupled excitable oscillators describing the cortex dynamics at a mesoscopic level, we discuss the possible nature of such a synchronization phase transition in structurally heterogeneous systems.

Primary author: BURIONI, Raffaella (University of Parma)

Presenter: BURIONI, Raffaella (University of Parma)

Session Classification: Wednesday session

Contribution ID: **38** Type: **Invited talk**

Scale-free correlations in the dynamics of a small ($N \sim 10000$) cortical network

Wednesday, September 21, 2022 9:00 AM (45 minutes)

The advent of novel opto-genetics technology allows the recording of brain activity with a resolution never seen before. The characterisation of these very large data sets offers new challenges as well as unique theory-testing opportunities. Here we discuss whether the spatial and temporal correlation of the collective activity of thousands of neurons are tangled as predicted by the theory of critical phenomena. The analysis shows that both the correlation length ξ and the correlation time τ scale as predicted as a function of the system size. With some peculiarities that we discuss, the analysis uncovers new evidence consistent with the view that the large scale brain cortical dynamics corresponds to critical phenomena.

Primary author: CHIALVO, Dante (Center for Complex Systems & Brain Sciences/ Universidad Nacional de San Martin, Argentina.)

Presenter: CHIALVO, Dante (Center for Complex Systems & Brain Sciences/ Universidad Nacional de San Martin, Argentina.)

Session Classification: Wednesday session

Contribution ID: **39** Type: **Regular talk**

Computing with memristive devices

Tuesday, September 20, 2022 12:10 PM (25 minutes)

The computing power of current digital hardware is hitting unavoidable physical limits.
Analog hardware has reemerged as an alternative solution for specialized applications.
In particular, neuromorphic computers, using combination of analog and digital elements, are becoming increasingly competitive in machine learning applications, offering high-speed, low-footprint, and low-power solutions.
Memristors are nonlinear history-dependent devices, and are key components in neuromorphic hardware.
In this talk I will summarize recent developments in the field and point towards fundamental open problems in analog computing with memristors.

Primary author: CARBAJAL, Juan Pablo (OST - Eastern Switzerland University of Applied Sciences)

Presenter: CARBAJAL, Juan Pablo (OST - Eastern Switzerland University of Applied Sciences)

Session Classification: Tuesday session

Contribution ID: **40** Type: **Regular talk**

Foundations of statistical mechanics for unstable interactions

Sunday, September 18, 2022 3:55 PM (25 minutes)

Traditional Boltzmann-Gibbs statistical mechanics does not apply to systems with unstable interactions, because for such systems the conventional thermodynamic limit does not exist. In unstable systems the ground state energy does not have an additive lower bound, i.e. no lower bound linearly proportional to the number N of particles or degrees of freedom. In this presentation (see [1] for details) unstable systems are studied whose groundstate energy is bounded below by a regularly varying function of N with index $\sigma \geq 1$. The index $\sigma \geq 1$ of regular variation introduces a classification with respect to stability. Stable interactions correspond to $\sigma = 1$. A simple example for an unstable system with $\sigma = 2$ is an ideal gas with a nonvanishing constant two-body potential. The foundations of statistical physics are revisited, and generalized ensembles are introduced for unstable interactions in such a way, that the thermodynamic limit exists. The extended ensembles are derived by identifying and postulating three basic properties as extended foundations for statistical mechanics: firstly, extensivity of thermodynamic systems, secondly, divisibility of equilibrium states, and thirdly statistical independence of isolated systems. The traditional Boltzmann-Gibbs postulate resp. the hypothesis of equal *a priori* probabilities are identified as special cases of the extended ensembles. Systems with unstable interactions are found to be thermodynamically normal and extensive. The formalism is applied to ideal gases with constant many-body potentials. The results show that, contrary to claims in the literature, stability of the interaction is not a necessary condition for the existence of a thermodynamic limit. As a second example, the formalism is applied to the Curie-Weiss-Ising model with strong coupling. This model has index of stability $\sigma = 2$. Its thermodynamic potentials, originally obtained in [2] are confirmed up to a trivial energy shift. The strong coupling model shows a thermodynamic phase transition of order 1 representing a novel mean-field universality class. The disordered high-temperature phase collapses into the ground state of the system. The metastable extension of the high-temperature free energy to low temperatures ends at absolute zero in a phase transition of order 1/2. Between absolute zero and the critical temperature of the first order transition all fluctuations are absent.

References

[1] Physical Review E, **105**, 024142 (2022).
[2] Physica A, **320**, 429 (2003).

Primary author: HILFER, Rudolf (Universitaet Stuttgart)

Presenter: HILFER, Rudolf (Universitaet Stuttgart)

Session Classification: Sunday session

Contribution ID: **41** Type: **Invited talk**

Quantum Theory of the Classical: Einselection, Envariance, and Quantum Darwinism

Monday, September 19, 2022 9:00 AM (45 minutes)

Core quantum postulates including the superposition principle and the unitarity of evolutions are natural and strikingly simple. I show that - when supplemented with a limited version of predictability (captured in the textbook accounts by the repeatability postulate) - these core postulates can account for all the symptoms of classicality. In particular, both objective classical reality and elusive information about reality arise, via quantum Darwinism, from the quantum substrate.

Primary author: Prof. ŻUREK, Wojciech (Los Alamos National Lab)

Presenter: Prof. ŻUREK, Wojciech (Los Alamos National Lab)

Session Classification: Monday session

Contribution ID: **42** Type: **Invited talk**

Emergence of Irreversibility and Hydrodynamic behavior from the Quantum Many-Body Dynamics: Experimental Evidence from Loschmidt Echoes and Related Experiment

Tuesday, September 20, 2022 11:15 AM (45 minutes)

The search for a justification and an appropriate description of irreversible macroscopic dynamics of fluids from time reversible mechanics was initiated Boltzmann, Loschmidt, Einstein and Smoluchowski. However, in spite of the impressive advances on both the experimental and progress addressing statistical nature, it has remained a polemic issue. Nowadays, the focus shifted towards the quantum dynamics mainly because of expectancies generated by the increasing number of qubits/spins handled on quantum information processing and the need for a match between the theory of gravitation with quantum mechanics. More than two decades ago we identified[1,2], at Córdoba, that Nuclear Magnetic Resonance could to address quantum signatures from spin diffusion and implement the time reversal procedures for an unlimited number of interacting spins. We realized that we could observe decoherence, irreversibility and the emergence of hydrodynamic behavior. With this purpose we developed a number of experimental strategies that generalized the one-body time reversal of the Spin Echo of Hahn. We dubbed this set of procedures as Loschmidt Echoes [3]. In this presentation I will review our experimental and theoretical quest to test our Central Hypothesis of Irreversibility [4]. According to this, and much as friction and dissipation results from reversible Newton equations, quantum dynamics of many-body systems far from equilibrium becomes decoherent, and hence irreversible in the thermodynamic limit of decreased interaction with the environment while the number of spins/qubits remains essentially infinite. Thus, in consistency with our most recent experimental findings [5,6], hydrodynamical irreversible behavior should result as an emergent property of reversible quantum dynamics.

[1] Quantum Dynamical Echoes in Spin Diffusion on Mesoscopic Systems.

HM Pastawski, PR Levstein and G Usaj, Phys. Rev. Lett. 75, 4310-4313 (1995)

[2] A Nuclear Magnetic Resonance answer to the Boltzmann-Loschmidt controversy?

HM Pastawski , G Usaj , PR Levstein, J Raya and J Hirschinger, Physica A 283 166 (2000)

[3] Loschmidt Echo, A Goussev, R Jalabert, HM Pastawski and D Wisniacki (2012) Loschmidt echo. Scholarpedia, 7(8):11687.

[4] Loschmidt echo in many-spin systems: a quest for intrinsic decoherence and emergent irreversibility. PR Zangara and H M Pastawski, Phys. Scr. 92 033001(2017)

[5] Perturbation independent decay of the Loschmidt echo in a many-spin system studied through scaled dipolar dynamics CM Sánchez, AK Chattah, KX Wei, L Buljubasich, P Cappellaro, and HM Pastawski, Phys. Rev. Lett. 124, 030601 (2020)

[6] Emergent decoherence induced by quantum chaos in a many-body system: A Loschmidt echo observation through NMR, CM Sánchez, AK Chattah, and HM Pastawski. Phys.Rev.A, 105, 052232 (2022), J. Magn. Res. (submitted)

Primary author: PASTAWSKI, Horacio (Academia Nacional de Ciencias)

Presenter: PASTAWSKI, Horacio (Academia Nacional de Ciencias)

Session Classification: Tuesday session

Contribution ID: **43** Type: **Regular talk**

Analytical Extension/Force curve of the Extensible Freely Jointed Chain Model (EFJC) and Worm-like Chain Model (EWLC)

Tuesday, September 20, 2022 10:20 AM (25 minutes)

Based on classical statistical mechanics, we calculate analytically the length extension under a pulling force of a polymer modeled as a freely jointed chain (FJC) with extensible bonds, the latter being considered as harmonic springs. We obtain an approximated formula for the extension curve that can reproduce with high precision the extension/force curves also at low values of the elastic constant of the spring, where previous phenomenological proposals differ substantially.

Moreover, a Transfer Matrix based procedure allowed to calculate numerically the extension/force curve of the polymer in the presence of both elastic contribution: the elastic longitudinal harmonic bonds giving the extensibility and the restoring bending between two consecutive bonds. In addition, an analytical expression has been found resulting in the most accurate approximation of the discrete extensible WLC model found at the date.

In all cases, we used the numerical experiments given by Langevin simulations to compare both the analytical results and the phenomenological expressions used in the literature.

Primary author: FIASCONARO, Alessandro (Department of Condensed Matter Physics and Institute for Biocomputation and Physics of Complex Systems, University of Zaragoza. Zaragoza, Spain.)

Co-author: Dr FALO, Fernando (Department of Condensed Matter Physics and Institute for Biocomputation and Physics of Complex Systems, University of Zaragoza. Zaragoza, Spain.)

Presenter: FIASCONARO, Alessandro (Department of Condensed Matter Physics and Institute for Biocomputation and Physics of Complex Systems, University of Zaragoza. Zaragoza, Spain.)

Session Classification: Tuesday session

Contribution ID: **44** Type: **Regular talk**

Multimodal approach in research on DNA damage

Saturday, September 17, 2022 5:15 PM (25 minutes)

Double-strand breaks (DSBs) of DNA are the most dangerous type of DNA lesions. Unrepaired DSBs may lead to cell death or cancer driving mutations. A deep understanding of the nature of DSBs, DSBs-related structural modifications of DNA, and repair process of DNA damage is critical to the maintenance of genomic integrity in all forms of life. In this presentation, a statistic-based approach for DNA double-strand breaks analysis based on the distribution of DNA fragments length derived from atomic force microscopy (AFM) images will be reported. The presented method relies on the fraction of the longest strands observed in the length distribution of DNA fragments, thus, it allows determining the accurate number of DSBs even in the case of limited image resolution [1]. DNA fragmentation was induced by the exposure to an anticancer chemotherapeutic drug, bleomycin (Blm). Moreover, the combination of AFM to visualize the products of DNA cleavage induced by Blm with their chemical characterization by SERS (surface-enhanced Raman spectroscopy) will be presented. An application of a statistical model enabled simultaneous analysis of AFM and SERS results and to observe a corelation of the conformational transition from B- to A-DNA with the decreasing average length of DNA fragments upon the bleomycin treatment [2]. Additionally, an application of SPM-based molecular nanospectroscopy, which poses a natural next step in characterization of local structural rearrangements of the DNA molecule exposed to damaging factors will be discussed.

Acknowledgements
This work is supported by the National Science Centre, Poland under the “OPUS 16” project (Reg. No. UMO-2018/31/B/ST4/02292).
References
[1] K. Sofińska, et al., Measurement, 198, 111362, 2022
[2] S. Seweryn, et al., Scientific Reports, 2022, accepted article

Primary author: SOFINSKA, Kamila (M. Smoluchowski Institute of Physics)

Presenter: SOFINSKA, Kamila (M. Smoluchowski Institute of Physics)

Session Classification: Saturday session

Contribution ID: **45** Type: **not specified**

Closing address

Wednesday, September 21, 2022 12:45 PM (15 minutes)

Session Classification: Wednesday session

Contribution ID: **46** Type: **not specified**

Welcome address

Saturday, September 17, 2022 2:45 PM (15 minutes)

Session Classification: Saturday session

Contribution ID: **47** Type: **Regular talk**

Crystalline phases with splay modulation in a system of hard wedges composed of balls

Monday, September 19, 2022 12:35 PM (25 minutes)

Computer simulation studies of equilibrium phases of matter play a crucial role in many fields, including biophysics, nanotechnology and soft matter science. They can be used as a guidance for synthesis of materials with desired properties. Of especially high interest are simple interaction models, which are easy to implement, but capture the most important characteristics of modelled molecules. Hard-core resuplsion is one of them. It was already proven years ago by Onsager, that a simple model of hard spherocylinders can capture isotropic-nematic phase transition. Since then, many types of hard molecules were studied and numerous purely entropic phase transitions were observed. In this study, we focus on hard wedges composed of tangent balls with linearly increasing radii. The molecule model possesses axial symmetry, but the up-down symmetry is broken ($C_{\infty v}$ symmetry group). The system is studied using Monte Carlo integration. Liquid phases in this model undergo Iso-N-SmA phase transition sequence, typical for elongated molecules. For a solid state, however, non-standard phases emerge. Apart from a non-polar hcp-like structure, two types of polar phases can be observed, where hexagonal clusters with a non-zero net polarization form periodic metastructures with splay modulation in the director field.

Primary authors: KUBALA, Piotr (Jagiellonian University); CIESLA, Michal (M. Smoluchowski Institute of Physics, Jagiellonian University, Kraków, Poland); LONGA, Lech (Jagiellonian University)

Presenter: KUBALA, Piotr (Jagiellonian University)

Session Classification: Monday session