

# 33rd M. Smoluchowski Symposium on Statistical Physics



## Report of Contributions

Contribution ID: 1

Type: poster

## Confinement-induced demixing and crystallization

Confinement occurs naturally in many physical, chemical and biological systems such as nanotubes, porous rocks or crowded living cells. The effect of confinement on the properties of simple liquids has therefore been carefully studied with experiments [1] and simulations [2,3] showing a large variety of interesting phenomena. Even for the simplest case of hard spheres confined between parallel, hard walls one observes spatially inhomogeneous density profiles and diffusivities [2], anisotropic structure factors [1], multiple-reentrant glass transitions [2] and solid-to-solid transitions between different crystalline phases [3].

Here we calculate the phase diagram of a mixture of size-disperse hard spheres in confinement by computer simulations and a statistical mechanics theory [4]. Despite the fact that this mixture is the prototypical model of a glass forming liquid, we find that when it is confined between walls, crystals form at densities significantly below the glass transition point. This crystallization is facilitated by fractionation, i.e., the demixing of particles based on their size. The numerical and theoretical results show semi-quantitative agreement, both featuring a novel honeycomb-shaped crystalline structure. We show that the crystallization can be exploited in a wedge geometry to demix particles of different sizes. Our findings could thus be exploited in the future as a purification technique.

### References

- [1] K. Nygård, R. Kjellander, S. Sarman, S. Chodankar, E. Perret, J. Buitenhuis and J. F. van der Veen, *Phys. Rev. Lett.* **108**, 037802 (2012)
- [2] S. Mandal, S. Lang, M. Gross, M. Oettel, D. Raabe, T. Franosch and F. Varnik, *Nat. Comm.* **5**, 4435 (2013)
- [3] M. Schmidt and H. Löwen, *Phys. Rev. Lett.* **76**, 4552 (1996)
- [4] G. Jung and C. F. Petersen, *Phys. Rev. Res.* **2**, 033207 (2020)

**Primary authors:** JUNG, Gerhard (University of Innsbruck); Dr PETERSEN, Charlotte F. (University of Innsbruck)

**Presenter:** JUNG, Gerhard (University of Innsbruck)

Contribution ID: 3

Type: **20 minute talk**

## Geometrical Optics of Constrained Brownian Motion

*Friday, December 4, 2020 9:50 AM (20 minutes)*

The optimal fluctuation method – essentially geometrical optics – gives a valuable insight into large deviations of constrained Brownian motion, and it achieves this purpose by simple means. I will illustrate these points by revisiting the Airy distribution - the probability distribution of the area under a Brownian excursion - and considering some additional statistics of Brownian excursions.

The geometrical optics immediately gives the large-area tail of the Airy distribution. It also predicts the position distribution of a Brownian excursion at an intermediate time, conditioned on a large area. Finally, it gives the area distribution on a sub-interval of Brownian excursion. The last two distributions exhibit dynamical phase transitions which have a simple geometric origin.

**Primary author:** MEERSON, Baruch (Hebrew University of Jerusalem)

**Presenter:** MEERSON, Baruch (Hebrew University of Jerusalem)

**Session Classification:** S4

Contribution ID: 4

Type: **20 minute talk**

## Biological Networks Regulating Cell Fate Choice Are Minimally Frustrated

*Friday, December 4, 2020 5:20 PM (20 minutes)*

Characterization of the differences between biological and random networks can reveal the design principles that enable the robust realization of crucial biological functions including the establishment of different cell types. Previous studies, focusing on identifying topological features that are present in biological networks but not in random networks, have, however, provided few functional insights. We use a Boolean modeling framework and ideas from the spin glass literature to identify functional differences between five real biological networks and random networks with similar topological features. We show that minimal frustration is a fundamental property that allows biological networks to robustly establish cell types and regulate cell fate choice, and that this property can emerge in complex networks via Darwinian evolution. The study also provides clues regarding how the regulation of cell fate choice can go awry in a disease like cancer and lead to the emergence of aberrant cell types.

**Primary author:** Prof. KESSLER, David (Bar-Ilan University)

**Co-authors:** Mr TRIPATHI, Shubham (Northeastern University); Prof. LEVINE, Herbert (Northeastern University)

**Presenter:** Prof. KESSLER, David (Bar-Ilan University)

**Session Classification:** S6

Contribution ID: 5

Type: **poster**

## Determination of psychotic behaviour using a network of chemical oscillators

*Thursday, December 3, 2020 6:21 PM (1 minute)*

Schizophrenia is the most common form of psychotic behaviour where patients experiences hallucination, dillusion or chaotic speech. Schizophrenia is difficult to detect and easily go undetected for years. Here we propose the idea of detecting schizophrenia by a network of interacting chemical oscillators. We optimized a classifier based on six interacting oscillator using genetic algorithm and obtained 82% accuracy of schizophrenia detection on a selected training dataset.

Keywords: Schizophrenia, EEG signal, chemical computing, oscillatory network, Oregonator model, genetic optimization

**Primary author:** Ms BOSE, Ashmita (Institute of Physical chemistry,Polish Academy of sciences)

**Co-author:** Prof. GORECKI, Jerzy (Institute of Physical chemistry,Polish Academy of Sciences)

**Presenter:** Ms BOSE, Ashmita (Institute of Physical chemistry,Polish Academy of sciences)

**Session Classification:** Poster Session

Contribution ID: 6

Type: 20 minute talk

## Diffusion limitations and translocation barriers in atomically thin biomimetic pores

*Friday, December 4, 2020 5:40 PM (20 minutes)*

Ionic transport in nano- to sub-nano-scale pores is highly dependent on translocation barriers and potential wells. These features in the free-energy landscape are primarily the result of ion dehydration and electrostatic interactions. For pores in atomically thin membranes, such as graphene, other factors come into play. Ion dynamics both inside and outside the geometric volume of the pore can be critical in determining the transport properties of the channel due to several commensurate length scales, such as the effective membrane thickness, radii of the first and the second hydration layers, pore radius, and Debye length. In particular, for biomimetic pores, such as the graphene crown ether we examine, there are regimes where transport is highly sensitive to the pore size due to the interplay of dehydration and interaction with pore charge. Picometer changes in the size, e.g., due to a minute strain, can lead to a large change in conductance. Outside of these regimes, the small pore size itself gives a large resistance even when electrostatic factors and dehydration compensate each other to give a relatively flat - e.g., near barrierless - free energy landscape. The permeability, though, can still be large and ions will translocate rapidly after they arrive within the capture radius of the pore. This, in turn, leads to diffusion and drift effects dominating the conductance. The current thus plateaus and becomes effectively independent of pore free energy characteristics. Measurement of this effect will give an estimate of the magnitude of kinetically-limiting features and experimentally constrain the local electromechanical conditions.

**Primary authors:** ZWOLAK, Michael (NIST); Dr SAHU, Subin (University of Colorado - Boulder)

**Presenter:** ZWOLAK, Michael (NIST)

**Session Classification:** S6

Contribution ID: 7

Type: **20 minute talk**

## Protein noise floor in gene expression: How cell growth and division contribute to it?

*Friday, December 4, 2020 5:00 PM (20 minutes)*

Gene expression in cells is a stochastic process. Experiments have shown that noise in protein levels does not decrease to zero as mean gene expression increases. The origins of the noise floor are still debated. The goal of our study was to check how several basic mechanisms affect the noise floor level. These mechanisms are: Cell-cycle dependent gene expression, translational bursting, random protein partitioning between daughter cells at division, and cell cycle desynchronization resulting in cell-cycle age distribution within the population. Our model gives analytical predictions of the existence of the noise floor and it semi-quantitatively reproduces the shapes of the experimental noise vs. protein concentration plots. We show what additional experimental information is needed for the mean-noise fitting to be unambiguous.

[1] J. Jędrak, A. Ochab-Marcinek, Contributions to the ‘noise floor’ in gene expression in a population of dividing cells, *Scientific Reports*, 10, 13533 (2020)

**Primary authors:** JĘDRAK, Jakub (Instytut Chemii Fizycznej PAN, ul. Kasprzaka 44/52, 01-224 Warszawa); OCHAB-MARCINEK, Anna (Institute of Physical Chemistry, Polish Academy of Sciences)

**Presenter:** OCHAB-MARCINEK, Anna (Institute of Physical Chemistry, Polish Academy of Sciences)

**Session Classification:** S6

Contribution ID: 8

Type: 20 minute talk

## Variational Approach to KPZ: Fluctuation Theorems, Large Deviation Function, and Probability Distribution Function

*Thursday, December 3, 2020 1:30 PM (20 minutes)*

The KPZ equation is - as known - a stochastic field theory that describes the kinetic roughening of surfaces and interfaces, plus many other nonequilibrium processes that belong to its universality class. For  $\lambda \neq 0$ , the systems described are intrinsically unstable and “lack of stationary probability distribution”. This can be readily inferred from the structure of the functional from which the deterministic KPZ equation stems in a variational formulation [1]. In fact, the time behavior of the aforementioned functional resembles that of a particle in a gravitational field [2]. A path-integral scheme has been set up in [3] that allows obtaining detailed and integral fluctuation theorems - as well as a Large Deviation Function for entropy production - for the KPZ equation, “regardless of the substrate dimensionality” [4]. After reviewing these issues, we close by discussing an explicit expression of the probability distribution for the KPZ system.

[1] H.S. Wio, “Variational formulation for the KPZ and related kinetic equations”, *Int. J. Bif. Chaos* 19, (2009) 2813-2821.

[2] H.S. Wio, M.A.Rodríguez, R.Gallego, J.A.Revelli, A. Ales and R.R.Deza, “d-Dimensional KPZ Equation as a Stochastic Gradient Flow in an Evolving Landscape: Interpretation and Time Evolution of Its Generating Functional”, *Front.Phys.*4 (2017): 52.

[3] H.S. Wio, R.R. Deza and J.A. Revelli, “Fluctuation theorems and large deviation functions in systems not featuring a steady state”, *J. Stat. Mech.* (2020) 024009.

[4] H.S. Wio, M.A. Rodríguez and R. Gallego, “Variational approach to KPZ: Fluctuation theorems and large deviation function for entropy production”, *Chaos* 30, (2020) 073107.

**Primary authors:** Prof. WIO, Horacio S. (Inst.Fisica Interdisc.&Sist.Compl.); Dr RODRIGUEZ, Miguel A. (Inst. Fisica Cantabria); Dr GALLEGO, Rafael (Mathematics Department); Dr DEZA, Roberto R. (IFIMAR); Dr REVELLI, Jorge A. (IFEG)

**Presenter:** Prof. WIO, Horacio S. (Inst.Fisica Interdisc.&Sist.Compl.)

**Session Classification:** S2

Contribution ID: 9

Type: **poster**

## Experimental study of the energy flux between two NESS thermostats.

*Thursday, December 3, 2020 6:20 PM (1 minute)*

We address the question of energy transport in out-of-equilibrium systems. The experiment consists in two coupled granular gas Non-Equilibrium Steady State (NESS) heat baths, in which 2 cm-scale rotors are imbedded. These Brownian-like mobiles are electro-mechanically coupled with a resistor  $R$ , allowing energy to flow between them. The mean flux is non-zero if the temperatures of the baths differ. The resistor  $R$  allows measurement of the flux and the temperatures in each bath simultaneously. Varying  $R$ , we show that, in the limit of non-dissipative coupling ( $R \rightarrow 0$ ), the heat flux obey the 'eXchange Fluctuation Theorem' (XFT), in a form proposed by Jarzynski and Wojcik in 2004, for the fluctuations of the flux between finite size equilibrium heat baths. This result, here obtained for granular gas thermostats experiment, is nevertheless representative of a large class of NESS systems.

**Primary author:** Dr NAERT, Antoine (ENS - Lyon, France)

**Presenter:** Dr NAERT, Antoine (ENS - Lyon, France)

**Session Classification:** Poster Session

Contribution ID: 10

Type: 20 minute talk

## Continuous time-reversal and the thermodynamic uncertainty relation

*Friday, December 4, 2020 1:20 PM (20 minutes)*

We introduce a continuous time-reversal operation which connects the time-forward and time-reversed trajectories in the steady state of an irreversible Markovian dynamics via a continuous family of stochastic dynamics. This continuous time-reversal allows us to derive a tighter version of the thermodynamic uncertainty relation (TUR) involving observables evaluated in different physical systems. Moreover, the family of dynamics realizing the continuous time-reversal contains an equilibrium dynamics halfway between the time-forward and time-reversed dynamics. We show that this equilibrium dynamics, together with an appropriate choice of the observable, turns the inequality in the TUR into an equality. We demonstrate our findings for the example of a two-dimensional rotational flow and discuss the role of the observable close to and far from equilibrium.

**Primary authors:** Dr DECHANT, Andreas (Department of Physics I, Kyoto University); Prof. SASA, Shin-ichi (Department of Physics I, Kyoto University)

**Presenter:** Dr DECHANT, Andreas (Department of Physics I, Kyoto University)

**Session Classification:** S5

Contribution ID: 11

Type: poster

## Steady oscillations in kinetic model of aggregation process with collisional fragmentation

Thursday, December 3, 2020 6:19 PM (1 minute)

In this work, we study a kinetic model of aggregation process with collisional fragmentation with use of two efficient implementations of numerical methods: direct simulation Monte Carlo and finite-difference scheme exploiting the low-rank matrix representations of the utilized kinetic coefficients. We concentrate our efforts on the analysis of the solutions for a particular class of non-local aggregation kernels

$K_{i,j} = i^a j^{-a} + i^{-a} j^a$ , with multiplicative expression for the fragmentation rates  $F_{i,j} = \lambda K_{i,j}$  with  $0 < \lambda \ll 1$ . For  $a > 0.5$  and  $\lambda < \lambda_c$  never-ending collective oscillations of the aggregates' concentrations take place [1].

The main contribution of this work is cross-validation of our previous observations with the utilization of the well-known stochastic acceptance-rejection method [2] and its modification to an accounting of the fragmentation events.

[1] Brilliantov N. V., Otieno W., Matveev S. A., Smirnov A. P., Tyrtysnikov E. E., Krapivsky P. L. (2018) // Steady oscillations in aggregation-fragmentation processes. *Physical Review E*, 98(1), 012109.

[2] Garcia A. L., Van Den Broeck C., Aertsens M., Serneels R. (1987) // A Monte Carlo simulation of coagulation. *Physica A: Statistical Mechanics and its Applications*, 143(3), 535-546.

**Primary authors:** Dr MATVEEV, Sergey (Skolkovo Institute of Science and Technology); Mr KALINOV, Aleksei (Skolkovo Institute of Science and Technology); Prof. KRAPIVSKY, Pavel (Boston University); Prof. BRILLIANTOV, Nikolai (Skolkovo Institute of Science and Technology)

**Presenter:** Dr MATVEEV, Sergey (Skolkovo Institute of Science and Technology)

**Session Classification:** Poster Session

Contribution ID: 12

Type: **poster**

## Energetics of critical oscillators in active bacterial baths

*Thursday, December 3, 2020 6:07 PM (1 minute)*

We investigate the nonequilibrium energetics near a critical point of a non-linear driven oscillator immersed in an active bacterial bath. At the critical point, we reveal a scaling exponent of the average power  $\langle \dot{W} \rangle \sim (D_a/\tau)^{1/4}$  where  $D_a$  is the effective diffusivity and  $\tau$  the correlation time of the bacterial bath described by Gaussian colored noise. Other features that we investigate are the average stationary power and the variance of the work both below and above the saddle-node bifurcation. Above the bifurcation, the average power attains an optimal, minimum value for finite  $\tau$  that is below its zero-temperature limit. Furthermore, we reveal a finite-time uncertainty relation for active matter, which leads to values of the Fano factor of the work that can be below  $2k_B T_{\text{eff}}$ , with  $T_{\text{eff}}$  the effective temperature of the oscillator in the bacterial bath. We analyze different Markovian approximations to describe the nonequilibrium stationary state of the system. Finally, we illustrate our results in the experimental context by considering the example of driven colloidal particles in periodic optical potentials within a E. Coli bacterial bath.

**Primary authors:** GOPAL, Ashwin (University of Luxembourg); ROLDAN, Edgar (Max Planck Institute for the Physics of Complex Systems); RUFFO, Stefano (SISSA)

**Presenter:** GOPAL, Ashwin (University of Luxembourg)

**Session Classification:** Poster Session

Contribution ID: 13

Type: 20 minute talk

## Extreme-Value Statistics of Stochastic Transport Processes

*Thursday, December 3, 2020 12:50 PM (20 minutes)*

We derive exact expressions for the finite-time statistics of extrema (maximum and minimum) of the spatial displacement and the fluctuating entropy flow of biased random walks. Our approach captures key features of extreme events in molecular motor motion along linear filaments. For one-dimensional biased random walks, we derive exact results which tighten bounds for entropy production extrema obtained with martingale theory and reveal a symmetry between the distribution of the maxima and minima of entropy production. Furthermore, we show that the relaxation spectrum of the full generating function, and hence of any moment, of the finite-time extrema distributions can be written in terms of the Marcinkiewicz-Pastur distribution of random-matrix theory. Using this result, we obtain efficient estimates for the extreme-value statistics of stochastic transport processes from the eigenvalue distributions of suitable Wishart and Laguerre random matrices. We confirm our results with numerical simulations of stochastic models of molecular motors.

**Primary author:** GUILLET, Alexandre

**Co-authors:** ROLDAN, Edgar (Max Planck Institute for the Physics of Complex Systems); Prof. JÜLICHER, Frank

**Presenter:** GUILLET, Alexandre

**Session Classification:** S2

Contribution ID: 14

Type: 20 minute talk

## Confined random motion: What is statistics? Gaussian or Laplacian?

*Thursday, December 3, 2020 1:10 PM (20 minutes)*

In biophysics, the single-particle tracking (SPT) is broadly used to quantify the kinetics of fluorescently-labelled molecules/proteins in live cells. This powerful tool in microscopy permits ones to resolve modes of motion of individual molecules for better understanding their role in such systems. The motion is not limited to pure (Brownian motion) diffusion, but directed, confined, anomalous diffusion are observed too. The study of their effects in live cells is of great interest.

Based on strict analytical calculations and simulations, we show that the confined motion in presence of Brownian motion in complex systems may have two different statistics. One of them has the normal distribution, whereas another, surprisingly, is under the Laplace distribution with fatter tails than the normal case (with thin tails always). Using the experimental data obtained from a recent SPT study on two particle types, G-protein coupled receptors and the G proteins with which the receptors interact, we have detected the normal and Laplace confinements. It is interesting that the contribution of the Laplace confinement is different for G proteins and receptors. The results are an important step to experimental cell probing and paves the way for a new strategy acting on the processes occurring in live cells through changing the confined motion of molecules into live cells, for example, by drugs. This analytic treatment can be used for different models, thus opening a new direction towards understanding the role of confinement in complex systems.

**Primary author:** STANISLAVSKY, Aleksander

**Presenter:** STANISLAVSKY, Aleksander

**Session Classification:** S2

Contribution ID: 15

Type: **poster**

## Electronic relaxation in solution: Exact solution of multi-state problems in time domain

*Thursday, December 3, 2020 6:08 PM (1 minute)*

Electronic relaxation in solution is an interesting phenomenon from experimental as well as theoretical point of view. This diffusion controlled process has been theoretically modeled by using Smoluchowski equation with a position dependent sink term. The problem has been solved for different potentials and sink functions. Single state problem where Smoluchowski equation for harmonic potential with a Dirac delta sink is the most general model which has been solved analytically in Laplace domain. Due to the complexity of equation, there is no time domain solution have been reported. In this work, we will give the exact analytical solution for this problem in time domain. We have solved one dimensional Smoluchowski equation for harmonic potential with a sink of ultra-short width. This problem has been solved for single state as well as two state model exactly in time domain. We have used Green's function method to solve the equation and calculated survival probability. For two state model, survival probability for both the states have been calculated explicitly. We have developed a general method to solve single state as well as coupled two state model which can be used to solve many similar problems.

**Primary author:** Ms MUDRA, Swati (Indian Institute of Technology Mandi, HP, India)

**Co-author:** Dr CHAKRABORTY, Aniruddha (Indian Institute of Technology Mandi, HP, India)

**Presenter:** Ms MUDRA, Swati (Indian Institute of Technology Mandi, HP, India)

**Session Classification:** Poster Session

Contribution ID: 16

Type: **poster**

## Search efficiency of (discrete) fractional Brownian motion in a random distribution of targets

*Thursday, December 3, 2020 6:09 PM (1 minute)*

Efficiency of search for randomly distributed targets is a prominent problem in many branches of the sciences. For the stochastic process of Lévy walks, a specific range of optimal efficiencies was suggested under variation of search intrinsic and extrinsic environmental parameters. We study fractional Brownian motion as a search process, which under parameter variation generates all three basic types of diffusion, from sub- to normal to superdiffusion. In contrast to Lévy walks, fractional Brownian motion defines a Gaussian stochastic process with power law memory yielding anti-persistent, respectively persistent motion. Computer simulations of this search process in a uniformly random distribution of targets show that maximising search efficiencies sensitively depends on the definition of efficiency, the variation of both intrinsic and extrinsic parameters, the perception of targets, the type of targets, whether to detect only one or many of them, and the choice of boundary conditions. We find that different search scenarios favour different modes of motion for optimising search success, defying a universality across all search situations. Some of our results are explained by a simple analytical model. Having demonstrated that search by fractional Brownian motion is a truly complex process, we propose an over-arching conceptual framework based on classifying different search scenarios. This approach incorporates search optimisation by Lévy walks as a special case.

**Primary authors:** JEBREIL KHADEM, Seyed Mohsen (Technische Universität Berlin); Prof. KLAPP, Sabine H.L. (Technische Universität Berlin); KLAGES, Rainer (Queen Mary University of London)

**Presenter:** JEBREIL KHADEM, Seyed Mohsen (Technische Universität Berlin)

**Session Classification:** Poster Session

Contribution ID: 17

Type: **poster**

## Efficiency of energy harvesting out of colored Lévy fluctuations, by a harmonic piezoelectric transducer

*Thursday, December 3, 2020 6:10 PM (1 minute)*

Based on studies where a linear piezoelectric energy harvester is subjected to external random mechanical excitations modeled through Gaussian noises (white and colored), it was decided to propose a more general colored noise of the Levy  $\alpha$ -stable type. Analytical, exact and approximate results and numerical results are presented on the characteristics of such excitations and the electrical power that can be extracted from them.

**Primary author:** GIULIANO, Martín E.

**Co-authors:** Dr SÁNCHEZ, Alejandro D.; Dr DEZA, Roberto R. (IFIMAR); Dr DEZA, J. Ignacio

**Presenter:** GIULIANO, Martín E.

**Session Classification:** Poster Session

Contribution ID: 18

Type: 20 minute talk

## Simple mathematical models for self-propelled motion on the water surface.

*Thursday, December 3, 2020 5:20 PM (20 minutes)*

Self-propelled motion on the water surface has fascinated scientists for almost two hundred years. There are many solid substances, such as camphor, camphene, and phenanthroline, which can develop to the water surface as a molecular layer, evaporate to the air phase and continuously dissolve into the water phase. This surface layer decreases the water surface tension and this decrease is local and time-dependent. Inhomogeneities in the surface concentration, resulting from fluctuations in release and evaporation, can break the symmetry around an object and drive its motion. The mathematical description of the self-propelled motion is complex because it should include object location, generated hydrodynamic flows, and dissipation of surface-active molecules. The simplest mathematical models consider the object position together with the concentration of surface-active molecules described by a reaction-diffusion equation in which the effective diffusion coefficient includes a hydrodynamic effect. However, there are many interesting examples of systems where the motion of a self-propelled object is strongly coupled with generated hydrodynamic flows and in such cases, the model mentioned above fails. We introduce another simple mathematical model that describes the time evolution of a self-propelled object on a liquid surface using such variables as the object location, the surface concentration of active molecules, and the hydrodynamic surface flow. The model is applied to simulate the time evolution of a rotor composed of a polygonal plate with camphor pills at its corners. We have qualitatively reproduced results of experiments, in which the inversions of rotational direction under periodic stop- and release- operations were investigated. The model correctly describes the probability of the inversion as a function of the duration of the phase when the rotor is stopped. Moreover, the model allows us to introduce the rotor asymmetry unavoidable in real experiments and study its influence on the studied phenomenon. Our numerical simulations have revealed that the probability of the inversion of rotational direction is determined by the competition among the transport of the camphor molecules by the flow, the intrinsic asymmetry of the rotor, and the noise amplitude.

**Primary author:** GORECKI, Jerzy (ICHF PAN)

**Co-authors:** Prof. KITAHATA, Hiroyuki; Prof. NAKATA, Satoshi; Dr KOYANO, Yuki

**Presenter:** GORECKI, Jerzy (ICHF PAN)

**Session Classification:** S3

Contribution ID: 19

Type: **poster**

## Exploring "inverse stochastic resonance" and nonstandard stochastic resonance with information-theoretic tools

*Thursday, December 3, 2020 6:11 PM (1 minute)*

Some pacemaker neurons show a depression of their mean firing rate for intermediate noise amplitudes, which reminds the response enhancement known as "stochastic resonance" (SR). Even though its analogy with SR goes no further, this phenomenon has been termed "inverse stochastic resonance" (ISR). In a recent work, the ISR phenomenon -as well as its close relative "nonstandard SR" (or more properly, noise-induced activity amplification, NIAA)- have been shown to stem from the weak-noise quenching of the initial distribution, in bistable regimes where the metastable state has a larger attraction basin than the global minimum. To further illustrate the mechanism whereby the ISR and NIAA phenomena take place, we revisit the one-variable model that led to that conclusion, exploring it with information-theoretic tools.

**Primary authors:** MARTINEZ, Nataniel (IFIMA-CONICET); Dr DEZA, Roberto R. (IFIMAR)

**Presenter:** MARTINEZ, Nataniel (IFIMA-CONICET)

**Session Classification:** Poster Session

Contribution ID: 20

Type: poster

## Phase transitions in the q-voter model with generalized anticonformity

Thursday, December 3, 2020 6:12 PM (1 minute)

Recent empirical studies provide evidence that so-called social hysteresis [1] is present in animal [1, 2, 3] as well as in human societies [4, 5, 6], which would suggest that (at least some) phase transitions observed in real social systems are discontinuous. It occurs that discontinuous phase transitions are not that typical in models of opinion dynamics. Within several versions of the  $q$ -voter model [7], belonging to the class of the binary-state dynamics [8, 9], only continuous phase transitions has been observed, including the original  $q$ -voter model [10] or the  $q$ -voter model with anticonformity [11]. However, the change of transition from continuous to discontinuous (for  $q > 5$ ) has been reported for the  $q$ -voter model with independence [11].

In [12] we introduce a  $q$ -voter model with generalized anticonformity. Previously it was assumed that the size of the unanimous group of influence needed for both conformity and anticonformity is equal [11]. We abandon this unjustified assumption and introduce a generalized model, in which the size of the influence group needed for conformity  $q_c$  and the size of the group needed for anticonformity  $q_a$  are independent variables and in general  $q_c \neq q_a$ .

We consider a system of  $N$  voters that form vertexes of an arbitrary network. Each of them is characterized by the dynamical binary variable  $S_i(t) = \pm 1$ ,  $i = 1, \dots, N$  which, in case of social systems, can be interpreted as an opinion on a given subject (yes/no, agree/disagree) at a given time  $t$ . In each elementary time step we randomly choose one agent that will reconsider its opinion. With probability  $p$  the chosen voter behaves like an anticonformist, whereas with complementary probability  $1 - p$  like a conformist. In any case we randomly choose a group of influence from the nearest neighbours of the agent without repetitions. The size of the group depends on the voter's response to social pressure ( $q_a$  for anticonformity,  $q_c$  for conformity). For  $q_a = q_c = q$  the model reduces to the original  $q$ -voter model with anticonformity introduced in [11]. If the group of influence is unanimous, the voter is influenced by the group and adapts to it (in case of conformity) or rebels against it (in case of anticonformity).

We analyse the model on a complete graph using linear stability analysis, numerical methods and Landau's theory. We calculate the analytical formulas for the lower spinodal and the tricritical point for which the phase transition changes from continuous to discontinuous. It has occurred that the generalized model displays both continuous and discontinuous phase transitions depending on the sizes of the groups of influence needed for conformity  $q_c$  and anticonformity  $q_a$ . If the parameter  $q_c$  is sufficiently larger than  $q_a$ , the type of the phase transition changes to discontinuous.

[1] Doering, G.N., Scharf, I., Moeller, H.V., Pruitt, J.N. *Social tipping points in animal societies in response to heat stress*. Nature Ecology and Evolution, 2(8):1298-1305, (2018)

[2] Beekman, M., Sumpter, D.J.T., Ratnieks, F.L.W. *Phase transition between disordered and ordered foraging in pharaoh's ants*. Proceedings of the National Academy of Sciences of the United States of America, 98(17):9703-9706, (2001)

[3] Pruitt, J.N., Berdahl, A., Riehl, C., Pinter-Wollman, N. and Moeller, H.V., Pringle, E.G., Aplin, L.M., Robinson, E.J.H., Grilli, J., Yeh, P., Savage, V.M., Price, M.H., Garland, J., Gilby, I.C., Crofoot, M.C., Doering, G.N., Hobson, E.A. *Social tipping points in animal societies*. Proceedings of the Royal Society B: Biological Sciences, 285(1887):20181282, (2018)

[4] Clark, A.E. *Unemployment as a Social Norm: Psychological Evidence from Panel Data*. Journal of Labor Economics, 21(2):323-351, (2003)

[5] Elster, J. *A Note on Hysteresis in the Social Sciences*. Synthese, 33(2/4):371-391, (1976)

- [6] Scheffer, M., Westley, F., Brock, W. *Slow response of societies to new problems: Causes and costs.* Ecosystems, 6(5):493-502, (2003)
- [7] Castellano, C., Muñoz, M.A., Pastor-Satorras, R. *Nonlinear q-voter model.* Physical Review E, 80(4):041129, (2009)
- [8] Gleeson, J.P. *Binary-state dynamics on complex networks: Pair approximation and beyond.* 3(2):021004, (2013)
- [9] Jędrzejewski, A., Sznajd-Weron, K. *Statistical Physics Of Opinion Formation: is it a SPOOF?* Comptes Rendus Physique, 20(4):244-261, (2019)
- [10] Castellano, C., Fortunato, S., Loreto, V. *Statistical physics of social dynamics.* Reviews of Modern Physics, 81(2):591-646, (2009)
- [11] Nyczka, P., Sznajd-Weron, K., Cisko, J. *Phase transitions in the q-voter model with two types of stochastic driving.* 86(1):011105, (2012)
- [12] Abramiuk, A., Pawłowski, J., Sznajd-Weron, K. *Is Independence Necessary for a Discontinuous Phase Transition within the q-Voter Model?* Entropy, 21:521, (2019)

**Primary author:** Mrs ABRAMIUK-SZURLEJ, Angelika (Wroclaw University of Science and Technology)

**Co-authors:** Mr PAWŁOWSKI, Jakub (Wroclaw University of Science and Technology); Prof. SZNAJD-WERON, Katarzyna (Wroclaw University of Science and Technology)

**Presenter:** Mrs ABRAMIUK-SZURLEJ, Angelika (Wroclaw University of Science and Technology)

**Session Classification:** Poster Session

Contribution ID: 21

Type: **poster**

## Numerical solution of temperature-dependent Smoluchowski equations

*Thursday, December 3, 2020 6:13 PM (1 minute)*

In this talk, we provide a numerical study of the recently developed generalised temperature-dependent Smoluchowski equations. To solve the new complex system, we adapt and improve the low-rank approach of solving large ODE systems. This allows us to quickly find approximate solutions for generalised systems of Smoluchowski equations even when the collision kernels change during aggregation. Our results confirm the analytical predictions of the temperature-dependent scaling, including analytically obtained scaling parameters. We also use a special type of Monte-Carlo simulations (temperature-dependent Monte-Carlo) to plot a phase diagram for different values of aggregation probability. We observe both temperature decrease and temperature increase scaling, as well as find more interesting behaviours at small system times.

**Primary author:** Mr OSINSKY, Alexander (Skolkovo Institute of Science and Technology)

**Co-author:** Prof. BRILLIANTOV, Nikolai (Skolkovo Institute of Science and Technology)

**Presenter:** Mr OSINSKY, Alexander (Skolkovo Institute of Science and Technology)

**Session Classification:** Poster Session

Contribution ID: 22

Type: poster

## Temperature-dependent Smoluchowski equations

*Thursday, December 3, 2020 6:06 PM (1 minute)*

We report a new class of Smoluchowski-like equations for ballistically aggregating particles in a space-uniform system. They naturally emerge when the derivation of the aggregation equations is performed starting from the Boltzmann kinetic equation for the mass-velocity distribution functions [1]. Then the system of equations for the zero-order moments of the distribution functions – the concentrations of aggregates of different size, corresponds to the conventional Smoluchowski equations. The aggregation rate coefficients of these equations depend on the second moments of the distribution function – partial temperatures of the aggregates. In this way, we obtain two coupled systems of equations – for the concentrations and temperatures [1]. We show that, depending on the aggregation probability, these equations provide two main types of scaling. The first one, when all collisions are aggregative leads to Smoluchowski-type evolution with a gradual decrease in temperature. The second one, when only a small fraction of collisions are aggregative, results in a stunning effect of the aggregation with temperature growth. We show that the temperature increase may be stable and perpetual until the system remains large enough for the notion of the temperature to persist. We also estimate the system parameters (restitution coefficient, aggregation probability), which can lead to this type of scaling. The theoretical results are confirmed by the numerical simulations.

[1] N. Brilliantov, T. Poeschel, and A. Formella, Increasing temperature of cooling granular gases, *Nature Communications*, 9 (2018) 797.

**Primary author:** Prof. BRILLIANTOV, Nikolai (Skolkovo Institute of Science and Technology)

**Co-authors:** Mr OSINSKY, Alexander (Skolkovo Institute of Science and Technology); Prof. FORMELLA, Arno (Department of Computer Science, University of Vigo); Prof. POESCHEL, Thorsten (Institute for Multiscale Simulation, Friedrich-Alexander-Universität Erlangen-Nürnberg)

**Presenter:** Prof. BRILLIANTOV, Nikolai (Skolkovo Institute of Science and Technology)

**Session Classification:** Poster Session

Contribution ID: 23

Type: **30 minute lecture**

## Galilean invariance for stochastic diffusive dynamics

*Friday, December 4, 2020 9:00 AM (30 minutes)*

Galilean invariance is a cornerstone of classical mechanics. It states that the equations of motion are the same in different inertial frames meaning they do not change under a Galilean transformation. Inertial frames, in turn, are reference frames describing closed systems where the frame-internal physics is not affected by frame-external forces. The description of real world systems, however, usually requires coarse-grained models integrating complex internal and external interactions indistinguishably as friction and stochastic forces, which intrinsically violates Galilean invariance. Starting from the Kac-Zwanzig Hamiltonian for a tracer particle in a heat bath of harmonic oscillators generating Brownian motion, we show how Galilean invariance is broken during the coarse graining procedure when deriving stochastic Langevin dynamics. We argue that traces of Galilean invariance survive for stochastic dynamics yielding a set of alternative rules, which we call weak Galilean invariance.

[1] A.Cairolì, R.Klages, A.Baule, Weak Galilean invariance as a selection principle for coarse-grained diffusive models, PNAS 115, 5714 (2018)

**Primary authors:** Dr CAIROLI, Andrea (Crick Institute); KLAGES, Rainer (Queen Mary University of London); BAULE, Adrian (Queen Mary University of London)

**Presenter:** KLAGES, Rainer (Queen Mary University of London)

**Session Classification:** S4

Contribution ID: 24

Type: 20 minute talk

## Random walks with asymmetric time delays

*Friday, December 4, 2020 10:30 AM (20 minutes)*

We study simple random-walk models with asymmetric time delays. Probability of a walker to move to the right or to the left depends on a difference between two state-dependent functions evaluated at states of the walker at two different times in the past. This might be seen as a model of a discrete replicator dynamics with strategy-dependent time delays. We assume hyperbolic-tangent fitness functions and to obtain analytical results we approximate them by step functions.

We observe a novel behavior. Namely, the mean position of the walker depends on time delays. This is a joint effect of stochasticity and time delays present in the system. In the deterministic version of a hyperbolic-tangent model, there appear symmetric cycles around a stationary point so the mean position of the walker stays the same. In stochastic versions without time delays, the expected value of the position of the walker is given by the stationary point.

If one interprets a position of the walker as a fraction of the population with a given strategy, then our results show that this fraction is a decreasing function of a delay, in fact a linear one for small delays. Moreover, bigger is the region with the (almost) unbiased random walk, smaller is the fraction of the population of the strategy with a bigger time delay.

**Primary authors:** Prof. MIĘKISZ, Jacek (University of Warsaw); Mr ŁOPUSZAŃSKI, Kamil

**Presenter:** Prof. MIĘKISZ, Jacek (University of Warsaw)

**Session Classification:** S4

Contribution ID: 26

Type: 20 minute talk

## Effective Langevin equations leading to large deviation function of time-averaged velocity for a nonequilibrium Rayleigh piston

*Friday, December 4, 2020 10:10 AM (20 minutes)*

We study fluctuating dynamics of a freely movable piston that separates an infinite cylinder into two regions filled with ideal gas particles at the same pressure but different temperatures. To investigate statistical properties of the time-averaged velocity of the piston in the long-time limit, we perturbatively calculate the large deviation function of the time-averaged velocity. Then, we derive an infinite number of effective Langevin equations yielding the same large deviation function as in the original model. Finally, we provide two possibilities for uniquely determining the form of the effective model.

**Primary author:** ITAMI, Masato (Nagoya University)

**Co-authors:** NAKAYAMA, Yohei (Tohoku University); NAKAGAWA, Naoko (Ibaraki University); SASA, Shin-ichi (Kyoto University)

**Presenter:** ITAMI, Masato (Nagoya University)

**Session Classification:** S4

Contribution ID: 27

Type: **20 minute talk**

## Modeling Echo Chambers and Polarization Dynamics in Social Networks

*Friday, December 4, 2020 12:40 PM (20 minutes)*

Echo chambers and opinion polarization recently quantified in several sociopolitical contexts and across different social media raise concerns on their potential impact on the spread of misinformation and on the openness of debates. Despite increasing efforts, the dynamics leading to the emergence of these phenomena remain unclear. We propose a model that introduces the dynamics of radicalization as a reinforcing mechanism driving the evolution to extreme opinions from moderate initial conditions. Inspired by empirical findings on social interaction dynamics, we consider agents characterized by heterogeneous activities and homophily. We show that the transition between a global consensus and emerging radicalized states is mostly governed by social influence and by the controversialness of the topic discussed. Compared with empirical data of polarized debates on Twitter, the model qualitatively reproduces the observed relation between users' engagement and opinions, as well as opinion segregation in the interaction network. Our findings shed light on the mechanisms that may lie at the core of the emergence of echo chambers and polarization in social media.

**Primary authors:** BAUMANN, Fabian (Humboldt University at Berlin); Dr LORENZ-SPREEN, Philipp (Max Planck Institute for Human Development); SOKOLOV, Igor (Humboldt University at Berlin); Dr STARNINI, Michele (Institute of Scientific Interchange, Turin)

**Presenter:** BAUMANN, Fabian (Humboldt University at Berlin)

**Session Classification:** S5

Contribution ID: 28

Type: 20 minute talk

## Symmetries and asymmetries of times to complete a chemical cycle

*Friday, December 4, 2020 1:00 PM (20 minutes)*

Measurements of durations of nonequilibrium stochastic processes provide valuable information on underlying microscopic kinetics and energetics. Theories for corresponding experiments to date are well-developed for single-particle systems only. Little is known for interacting systems in nonequilibrium environments. We introduce and discuss a basic model for cycle processes interacting with an environment that can be out of thermodynamic equilibrium. We find a surprising richness of cycle time variations with environmental conditions. This manifests itself in unequal cycle times in forward and backward cycle directions, speeding up of backward cycles by interactions, and dynamical phase transitions, where cycle times become multimodal functions of a bias. The model allows us to relate these effects to specific microscopic mechanisms, which can be helpful for interpreting experiments.

**Primary authors:** RYABOV, Artem (Charles University); VORÁČ, David (Charles University); LIPS, Dominik (Universität Osnabrück); MAASS, Philipp (Universität Osnabrück)

**Presenter:** RYABOV, Artem (Charles University)

**Session Classification:** S5

Contribution ID: 29

Type: 20 minute talk

## Anomalous Diffusion and Generalized Cattaneo Equation

*Friday, December 4, 2020 9:30 AM (20 minutes)*

The generalized Cattaneo equation (GTE) involving memory effect is introduced by smearing the time derivatives. Consistency conditions which the smearing functions obey restrict freedom in their choice. The proposed scheme goes beyond the approach based on using fractional derivatives. I present the conditions under which solutions of the GTE can be recognized as probability distribution, i.e. are normalizable and nonnegative on their domain.

**Primary author:** GORSKA, Katarzyna (Institute of Nuclear Physics, Polish Academy of Sciences)

**Presenter:** GORSKA, Katarzyna (Institute of Nuclear Physics, Polish Academy of Sciences)

**Session Classification:** S4

Contribution ID: 30

Type: poster

## Combinatorial aspects of the scattering on the Dirac delta potential

*Thursday, December 3, 2020 6:14 PM (1 minute)*

We study a system where a particle scatter on the periodic Dirac delta potential. The problem is canonical i.e. it is considered during typical quantum mechanics course. There are several approaches to solve the Schrodinger equation for such a systems [1] [2]. However most of solutions rely on different matrix method. We would like to introduce new, combinatorial method by writing system of recursive equations. Based off this solution we write transmission and reflected coefficients of a wave functions of a particle, which is the common way to describe Quantum tunnelling.

The most interesting conclusion from the introduced technique: we reveal combinatorial structure of the typical quantum mechanics problem and write transmission and reflected coefficients using binomial coefficients as the number of combinations with repetition.

[1] Fatih Erman, Manuel Gadella, and Haydar Uncu. On scattering from the one dimensional multiple dirac delta potentials. *European Journal of Physics*, 39, 01 2018

[2] D. Kiang. Multiple Scattering by a Dirac Comb. *American Journal of Physics*, 42:785–787, September 1974.

**Primary authors:** NOWAK, Przemysław (Warsaw University of Technology, Faculty of Physics); Dr SIUDEM, Grzegorz (Warsaw University of Technology, Faculty of Physics)

**Presenter:** NOWAK, Przemysław (Warsaw University of Technology, Faculty of Physics)

**Session Classification:** Poster Session

Contribution ID: 31

Type: 20 minute talk

## The q-voter model with attractive and repulsive interactions and independence on random graphs

*Friday, December 4, 2020 12:20 PM (20 minutes)*

The  $q$ -voter model with both attractive (roughly speaking, ferromagnetic-like) and repulsive (antiferromagnetic-like) interactions on random graphs is investigated. In this model the agent, represented by a two-state spin located in a node of a graph, with probability  $1 - p$  changes his/her opinion under the influence of a clique of  $q$  randomly chosen neighbors and with probability  $p$  acts independently and changes opinion randomly. In the former case the agent changes opinion if opinions of all selected neighbors interacting with him/her attractively via the attached edges of the graph ("friends") are opposite and simultaneously opinions of all selected neighbors interacting with him/her repulsively ("disliked persons") are the same as the agent's one. The parameter  $p$  measures the level of stochastic noise in the model. For  $q \geq 4$  the model on graphs with large mean degree of nodes exhibits first-order ferromagnetic transition with decreasing  $p$ , with a clearly visible hysteresis loop. The width of this loop decreases with increasing fraction of the repulsive interactions and the transition can eventually become second-order. For  $q < 4$  the transition is always second-order. An extension of the pair approximation taking into account presence of the repulsive interactions predicts quantitatively well results of Monte Carlo simulations of the model in a broad range of parameters.

**Primary author:** Dr KRAWIECKI, Andrzej (Faculty of Physics, Warsaw University of Technology)

**Presenter:** Dr KRAWIECKI, Andrzej (Faculty of Physics, Warsaw University of Technology)

**Session Classification:** S5

Contribution ID: 32

Type: poster

## Photoluminescence of Complex Systems

Thursday, December 3, 2020 6:05 PM (1 minute)

The photoluminescence degradation of the thermally evaporated Alq3 thin films can be described by a four components model based on the Kohlrausch-Williams-Watt (KWW) function. This model improved the agreement between experimental data and the theoretical fit with respect to the four components model based on “pure” exponential functions. In fact, the negative bump in PL intensity decay observed in the reference not-annealed sample is perfectly fitted, and the last part of the time resolved spectroscopy improved its adherence to experimental data both in annealed and not-annealed samples.

A material frame of reference has been introduced in order to investigate the physical nature of the KWW function in relaxation processes and at the same time, explain the peculiar experimental features emerged in the time-spectral PL behaviour. The introduction of a nonlinear time variable, named material clock or material time, overcomes the difficulties carried by the anomalous behaviour considering the process from a bare point of view: the relaxation behaves ideally whereas the material frame of reference is going to be stretched or compressed. This allows to model the PL degradation dynamics as a damped harmonic oscillator. Once the physics has been understood, it is possible to restore the laboratory frame of reference and define the reduced mass, a time-dependent function that unlocks the physical meaning of the experimental peculiarities observed in the PL emission.

The results are framed in the context of physical-chemical reactions in order to emphasize how the KWW function is a sum of sub-processes. The physical meaning of these sub-processes can be related to internal and environmental agents interactions under defined physical conditions. These insights highlight the usefulness of the proper mathematical procedures and properties, such as the monotonicity and the complete monotonicity, for investigating the PL emission of this organometallic molecule. Moreover, this method is also promising for describing the photoluminescent processes of similar organic molecules both for basic research and optoelectronic applications.

**Primary author:** LATTANZI, Ambra (Institute of Nuclear Physics IFJ-PAN, Kraków, Poland - ENEA FSN-FUSPHYS-TSM, Frascati (Rome), Italy)

**Co-authors:** Prof. DATTOLI, Giuseppe (ENEA FSN-FUSPHYS-TSM, Frascati (Rome), Italy); Prof. BALDACCHINI, Giuseppe

**Presenter:** LATTANZI, Ambra (Institute of Nuclear Physics IFJ-PAN, Kraków, Poland - ENEA FSN-FUSPHYS-TSM, Frascati (Rome), Italy)

**Session Classification:** Poster Session

Contribution ID: 33

Type: **poster**

## **Cyclic Kuramoto models and Byzantine attack**

*Thursday, December 3, 2020 6:15 PM (1 minute)*

Cyclic, one-dimensional Kuramoto models with various types of interactions are reviewed. Ruch models are less resilient to Byzantine perturbations than a classic solution would suggest.

**Primary author:** GÓRA, Paweł (Jagiellonian University)

**Presenter:** GÓRA, Paweł (Jagiellonian University)

**Session Classification:** Poster Session

Contribution ID: 34

Type: poster

## The study of structure influence on diffusion across alginate membranes filled with magnetite

Thursday, December 3, 2020 6:16 PM (1 minute)

The combination of polymer and inorganic substance in hybrid membrane results in favourable selectivity and permeability, and consequently such membrane becomes a promising alternative to conventional membrane materials. The resulting membranes show improved chemical, mechanical, and thermal stability and hydrophilic–hydrophobic balance. The objective of this research is to determine whether there is a relation between membrane morphology, which is characterized by different parameters, and the diffusive transport in the membrane. We expect that different amount of magnetite particles in alginate matrix cross-linked by different agents influence on structure and morphology properties and also affects the diffusion and transport properties. In this work, we investigate the morphology of cross-sections of the hybrid alginate membranes filled with various amount of magnetite ( $Fe_3O_4$ ) and crosslinked using four different agents: calcium chloride, phosphoric acid, glutaraldehyde and citric acid. A key aspect of showing structure - diffusion relationship can be the study of the simulation of particle motion in a membrane environment, and in our case, it is a simulation of a random walk on the structures of hybrid alginate membranes. For a better understanding of the problem, we model structures of two-dimensional heterogenic membranes which resemble real structures and then simulate random walk on them. The prototype structures of hybrid polymeric membranes are created with the desired quantity, size and distribution of obstacles, which corresponds to the given amount of magnetite in the hybrid alginate membrane. Generated membranes possessing specific parameters are comparable to the real hybrid alginate membranes filled with magnetite and give a real chance to find the relation between diffusion and structure properties. This observation may support a better understanding of structure influence on mass transport through polymer materials.

[1] G. Dudek, M. Krasowska, R. Turczyn, M. Gnus, A. Strzelewicz, Structure, morphology and separation efficiency of hybrid Alg/ $Fe_3O_4$  membranes in pervaporative dehydration of ethanol, Separation and Purification Technology 182 (2017) 101–109

[2] M. Krasowska, A. Strzelewicz, G. Dudek, M. Cieřła, Structure-diffusion relationship of polymer membranes with different texture, Physical Review E 95, 012155 (2017)

[3] A. Strzelewicz, M. Krasowska, G. Dudek, M. Cieřła, Design of polymer membrane morphology with prescribed structure and diffusion properties, Chemical Physics, 531, 110662 (2020)

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

**Presenter:** STRZELEWICZ, Anna (Silesian University of Technology)

**Session Classification:** Poster Session

Contribution ID: 36

Type: 20 minute talk

## The role of ergotropy in the quantum thermodynamics

*Friday, December 4, 2020 1:40 PM (20 minutes)*

Ergotropy is a state function of a density matrix which physical interpretation is the optimal work that can be extracted through the arbitrary unitary channel. The concept naturally appears in frameworks with implicit work reservoirs (e.g. external fields modeled by time-dependent Hamiltonians), where, in particular, the process of charging and discharging of so-called quantum batteries is studied. We reveal that the same quantity appears in autonomous systems with an idealized model of the work reservoir - a quantum weight. Despite similarities between those two approaches, we reveal a fundamental difference, namely the emergence of the locked energy in coherences, i.e. the quantum part of the state that contributes to ergotropy but cannot be extracted as a work. Furthermore, we prove the relation between the ergotropy and free energy, where the former can be interpreted as a generalization of the latter for systems coupled to finite-size heat baths, such that in the thermodynamic limit the total ergotropy of the system and the heat bath approaches the free energy. As a consequence, we derive the second kind of locked energy, due to the finite-size of the bath, which is given by the difference of free energy between the global passive state and the corresponding equilibrium state.

**Primary author:** Dr ŁOBEJKO, Marcin (University of Gdansk)

**Presenter:** Dr ŁOBEJKO, Marcin (University of Gdansk)

**Session Classification:** S5

Contribution ID: 37

Type: 20 minute talk

## Spontaneous symmetry breaking of active phase in coevolving nonlinear voter model

*Friday, December 4, 2020 12:00 PM (20 minutes)*

A feedback loop between the network topology and dynamical processes that occur between nodes is common in real-world networks. The topology impacts the evolution of node states, which in turn influence the way the structure itself is modified. This feedback is a signature of networks that are called adaptive or coevolutionary. Adaptive networks are especially relevant for social systems, where they can model phenomena such as the emergence of consensus and polarization, opinion formation, or group fragmentation. These coevolutionary models rely on two basic mechanisms. One accounts for the changes in the node states, whereas the other for the link rewiring. Both of them may be implemented in various ways. The voter model, as a minimalist model of opinion formation process, provides the basis for the evolution of state variables in many adaptive networks that represent social interactions. Being analytically tractable, it has played a fundamental role in understanding the process of network fragmentation. This work extends the study in this area by the analysis of one of the nonlinear extensions of the coevolving voter model.

In the analyzed model, each node in the network represents a voter and can be in one of two states that correspond to different opinions shared by the voters. A voter disagreeing with its neighbor's opinion may either adopt it or rewire its link to another randomly chosen voter with any opinion. The system is studied by means of the pair approximation in which a distinction between the average degrees of nodes in different states is made. This approach allows us to identify two dynamically active phases: a symmetric and an asymmetric one. The asymmetric active phase, in contrast to the symmetric one, is characterized by different numbers of nodes in the opposite states that coexist in the network. The pair approximation predicts the possibility of spontaneous symmetry breaking, which leads to a continuous phase transition between the symmetric and the asymmetric active phases. In this case, the absorbing transition occurs between the asymmetric active and the absorbing phases after the spontaneous symmetry breaking. Discontinuous phase transitions and hysteresis loops between both active phases are also possible. Interestingly, the asymmetric active phase is not displayed by the model where the rewiring occurs only to voters sharing the same opinion, studied by other authors. Our results are backed up by Monte Carlo simulations.

During the talk, we will compare both the versions of the model, and we will see how a seemingly small difference in the link rewiring dynamics leads to profound differences in the phase diagrams exhibited by the models.

**Primary authors:** JĘDRZEJEWSKI, Arkadiusz (Wrocław University of Science and Technology); Mrs TORUNIEWSKA, Joanna (Warsaw University of Technology); Dr SUCHECKI, Krzysztof (Warsaw University of Technology); Dr ZAIKIN, Oleg (ITMO University); Prof. HOŁYST, Janusz (Warsaw University of Technology)

**Presenter:** JĘDRZEJEWSKI, Arkadiusz (Wrocław University of Science and Technology)

**Session Classification:** S5

Contribution ID: 38

Type: **poster**

## Kramers-like problem for underdamped Levy flights

Thursday, December 3, 2020 6:02 PM (1 minute)

The noise driven motion in a bistable potential acts as the archetypal model of various physical phenomena. In the weak noise limit, for the overdamped particle driven by a non-equilibrium,  $\alpha$ -stable noise the ratio of forward and backward transition rates depends only on the width of the potential barrier separating both minima. The poster presents analytical and numerical results showing that in the regime of full dynamics the ratio of transition rates depends both on widths and heights of the potential barrier separating minima of the double-well potential.

K. Capała and B. Dybiec, *Underdamped, anomalous kinetics in double-well potentials*, Phys. Rev. E **102**, 052123 (2020).

**Primary authors:** Mr CAPAŁA, Karol (Institute of Theoretical Physics, Jagiellonian University); Prof. DYBIEC, Bartłomiej (Institute of Theoretical Physics, Jagiellonian University)

**Presenter:** Mr CAPAŁA, Karol (Institute of Theoretical Physics, Jagiellonian University)

**Session Classification:** Poster Session

Contribution ID: 40

Type: poster

## Diffusion-controlled reactions: Extension of time-dependent Smoluchowski's rate coefficient to reactions in media with relaxation

Thursday, December 3, 2020 6:17 PM (1 minute)

Processes involving Brownian motion of small reactants toward much larger static particles (sinks) and subsequent trapping of these reactants by the sinks are very commonly encountered in both nature and in artificial media. Theoretically these processes are described by so-called trapping model of the irreversible bulk diffusion-controlled reactions. To avoid difficulties of classical diffusion theory the hyperbolic diffusion approximation is often used [1, 2]. Within the scope of the telegrapher equation the density distribution of reactants  $\rho(r, t)$  about a spherical sink of radius  $R$  obeys the initial boundary-value problem with Smoluchowski's condition on the reaction surface [1]. The primary task for the theory of diffusion-controlled reactions is the calculation of the reaction rate coefficient:

$$k(t) = k_S \frac{R}{\tau_d} \int_0^t \exp\left(-\frac{t-\zeta}{\tau_d}\right) \left. \frac{\partial \rho(r, \zeta)}{\partial r} \right|_{r=R} d\zeta.$$

Hereafter  $k_S = 4\pi RD$  is the Smoluchowski steady state rate coefficient;  $\tau_d$  and  $D$  are the relaxation time for the gradients of density distribution of reactants and diffusion coefficient, respectively. We solved the posed problem exactly and, using expression (1), for the time-dependent reaction rate coefficient obtained

$$k(t) = k_S \left\{ \left[ 1 - \exp\left(-\frac{t}{\tau_d}\right) \right] + \frac{R}{\sqrt{\tau_d D}} \left[ \exp\left(-\frac{t^2}{2\tau_d}\right) I_0\left(\frac{t^2}{2\tau_d}\right) - \exp\left(-\frac{t}{\tau_d}\right) \right] \right\},$$

where  $I_0(z)$  is the first kind modified Bessel function of order zero. It is important to note that the last term in expression (1) was erroneously omitted in the relevant formula derived by Rice (see expression (289) in page 330 of book [1]). Formula (2) generalizes the classical Smoluchowski result to short time values, which is important for reactions occurring in media with relaxation [2].

[1] S. A. Rice, Diffusion-limited reactions, Amsterdam: Elsevier, 1985.

[2] D. Jou, J. Casas-Vazquez and G. Lebon, Extended irreversible thermodynamics (Fourth Edition), Springer, 2010.

**Primary author:** Prof. TRAYTAK, Sergey (N.N. Semenov Federal Research Center for Chemical Physics, Russian Academy of Sciences)

**Presenter:** Prof. TRAYTAK, Sergey (N.N. Semenov Federal Research Center for Chemical Physics, Russian Academy of Sciences)

**Session Classification:** Poster Session

Contribution ID: 41

Type: **30 minute lecture**

## On zero-delay synchronization in a network of timed automata modeling cardiac tissue

Friday, December 4, 2020 4:30 PM (30 minutes)

A network of timed automata (NTA), inspired by Greenberg-Hastings cellular automata, can efficiently and faithfully reflect the work of the real pacemaker [1]. In this system, each automaton cyclically switches between three states of a certain length of time: from  $F$  firing state of length  $f$ , to  $R$  refractory state of length  $r$  and then to  $A$  activity state of length  $a$ , what closely follows the phenomenologically known oscillations of myocytes. As a result of interactions between neighboring cells, the self-organization of the oscillating units to a common oscillation emerges which then leads to forming a signal of initiating a contraction of the whole heart. Thus NTA establishes an appropriate platform to model a natural human pacemaker, in which we gain insight into conditions and stages of the synchronization process [2].

The visible effect of synchronization in NTA is the excitation wave, i.e. the emergence of steady move of a cluster formed by automata staying in  $F$  state.

The synchronization can be of frequency locking type, when some automata force the neighboring automata to faster switch the state  $A$  to  $F$  than it is expected by intrinsic automaton's cycle, or of phase-locking type, when neighboring automata exhibit the common difference in oscillatory phase. Thus, the frequency-locking synchronizations result in the fast rhythms. The visible effect of such synchronization is a spiral origin of the excitation wave. The phase-locking synchronization occurs when neighboring automata are one step late in the advancement of the cyclic transitions of intrinsic time periods. A visible effect of such synchronization is propagation of the excitation wave with rhythm comparable to the period of oscillating automata.

The strength of synchronization is due to the reduction of uncorrelated degrees of freedom to a collective mode of operation, which then enables the long-term ordering and coordination of biological processes

The emergence of zero-delay phase-locking synchronization, the marching squad synchronization, has been observed in NTA when in response to the  $F$  state of neighbors, the length of the refractory phase  $r$  was increased [1].

On the other hand, in NTA system in which the vagal regulation was modeled as increase in the length  $a$  of the activity state in response to the vagal activity, such synchronization is also observed but only when the activity of vagal system often changes [2].

The mechanisms behind synchronizing without any delay in spatially distributed systems are not clear and debated. The presentation will be devoted to analyze possible mechanisms leading to the marching squad synchronization in the NTA system modeling the pacemaker.

[1] D. Makowiec "Pacemaker rhythm through networks of pacemaker automata - a review" Acta Physica Polonica B Proceedings Supplement, 7(2014) 347

[2] D. Makowiec, W. Miklaszewski, J. Wdowczyk, A. Lawniczak "From cellular automata model of vagal control of human right atrium to heart beats patterns" Physica D, to appear, (2020)

**Primary author:** MAKOWIEC, Danuta (Institute of Theoretical Physics, University of Gdańsk)

**Presenter:** MAKOWIEC, Danuta (Institute of Theoretical Physics, University of Gdańsk)

**Session Classification:** S6

Contribution ID: 45

Type: **30 minute lecture**

## Spectral content of a single trajectory

*Thursday, December 3, 2020 10:30 AM (30 minutes)*

In this presentation I will overview a recent progress in the theoretical, numerical and experimental analyses of spectral densities of individual random trajectories of a finite length. On example of a broad class of anomalous diffusions - the so-called fractional Brownian motion, I will demonstrate that one may calculate analytically the full probability density function of such random functionals, parametrised by a frequency and a finite observation time, and extract a very meaningful information on the evolution of a process under study. In particular, I will show that the large frequency behaviour of the coefficient of variation of this distribution provides a robust criterion of anomalous diffusion, which analytical prediction is validated by a comparison with experiments on dynamics in live cells and in agarose hydrogels, and also by extensive numerical simulations. If time permits, I will also discuss the peculiarities of spectra in out-of-equilibrium systems, as exemplified by a Brownian Gyrotator model, and also of the so-called active Brownian motion.

**Primary author:** OSHANIN, Gleb (Theoretical Condensed Matter, Sorbonne Universités / CNRS)

**Presenter:** OSHANIN, Gleb (Theoretical Condensed Matter, Sorbonne Universités / CNRS)

**Session Classification:** S1

Contribution ID: 46

Type: **30 minute lecture**

## Optimization and Growth in First-Passage Resetting

*Thursday, December 3, 2020 4:00 PM (30 minutes)*

We combine resetting and first-passage to define “first-passage resetting”, where a random walk is reset to a fixed position due to a first-passage event of the walk itself. On the infinite half-line, first-passage resetting of isotropic diffusion is non-stationary, in which the number of resetting events grows with time as  $t^{1/2}$ . We calculate the resulting spatial probability distribution of the particle, and also obtain this distribution by a path decomposition approach. In a finite interval, we define an first-passage-resetting optimization problem that is motivated by reliability theory. Here, the goal is to operate a mechanical system close to its maximum capacity without experiencing too many breakdowns. When a breakdown occurs, the system is reset to its minimal operating point. We define and optimize an objective function that maximizes the reward (being close to maximum operation) minus a penalty for each breakdown. Finally, we study a first-passage-driven domain growth dynamics in which its boundary recedes by a specified amount when a diffusing particle reaches the boundary, after which resetting occurs. We find a wide range of dynamical behaviors for the domain growth rate in the interval and the semi-infinite line.

**Primary authors:** REDNER, Sidney (Santa Fe Institute); DE BRUYNE, Benjamin (Perimeter Institute of Theoretical Physics); Prof. RANDON-FURLING, Julien (Université Paris 1 Panthéon Sorbonne)

**Presenter:** REDNER, Sidney (Santa Fe Institute)

**Session Classification:** S3

Contribution ID: 47

Type: **30 minute lecture**

## Super-spreaders in the Corona Epidemics

*Thursday, December 3, 2020 9:00 AM (30 minutes)*

Recently a powerful example of a replicating nano-machinery entered our society. In principle it's just a normal disease, that one attempt to model with 3 or 4 simple coupled equations with 2 important parameters: a timescale, and a replication factor (the famous  $R_0$ ). And then one try to guess how changes in society changes  $R_0$  and perhaps adopt some more or less strong lock-down measures. However, this virus have more "personality" than that. It behaves different in different persons, and persons behave differently. Presumably only a few of us infect a lot, while most does not infect so much. This assumption is supported by the observation that couples living together only infect each other with about 15 percent probability, indicating that most infected people are not really infectious. I will discuss this and other aspects of Covid-19 in perspective of models that describe heterogeneous individuals in a society. In particular we suggest that limiting superspreading opportunities is a cost effective strategy to mitigate Covid-19.

**Primary author:** Prof. SNEPPEN, Kim (Niels Bohr Institute)

**Presenter:** Prof. SNEPPEN, Kim (Niels Bohr Institute)

**Session Classification:** S1

Contribution ID: 48

Type: **30 minute lecture**

## Restart: The Physics Of Starting Anew

*Thursday, December 3, 2020 4:30 PM (30 minutes)*

Stopping a process in its midst—only to start it all over again—may prolong, leave unchanged, or even shorten the time taken for its completion. Among these three possibilities, the latter is particularly interesting as it suggests that restart can be used to expedite the completion of complex processes involving strong elements of chance. This turned out to be important in computer science where restart drastically improves performance of randomized algorithms, but is not less relevant to many physical, chemical, and biological processes where restart plays a central role. In this talk, I will provide an introduction to the theory of restart phenomena and review some of its applications in statistical, chemical, and biological physics.

### References

- [1] S. Reuveni, Phys. Rev. Lett. **116**, 170601 (2016).
- [2] A. Pal & S. Reuveni, Phys. Rev. Lett. **118**, 030603 (2017).
- [3] A. Pal, I. Eliazar & S. Reuveni, Phys. Rev. Lett. **122**, 020602 (2019).
- [4] S. Ray, D. Mondal & S. Reuveni, J. Phys. A. **52**, 255002 (2019).
- [5] S. Ray & S. Reuveni, J. Chem. Phys. **152**, 234110 (2020).
- [6] O. T. Friedman, A. Pal, A. Sekhon, S. Reuveni & Y. Roichman, J. Phys. Chem. Lett. **11**, 7350 (2020).
- [7] A. Pal, Ł. Kuśmierz & S. Reuveni, Phys. Rev. Research **2**, 043174 (2020).

**Primary author:** REUVENI, Shlomi (Tel Aviv University)

**Presenter:** REUVENI, Shlomi (Tel Aviv University)

**Session Classification:** S3

Contribution ID: 49

Type: **30 minute lecture**

## Packets of diffusing particles exhibit universal exponential tails

*Thursday, December 3, 2020 12:00 PM (30 minutes)*

Brownian motion is a Gaussian process described by the central limit theorem. However, exponential decays of the positional probability density function  $P(X, t)$  of packets of spreading random walkers, were observed in numerous situations that include glasses, live cells, and bacteria suspensions. We show that such exponential behavior is generally valid in a large class of problems of transport in random media. By extending the large deviations approach for a continuous time random walk, we uncover a general universal behavior for the decay of the density [1]. It is found that fluctuations in the number of steps of the random walker, performed at finite time, lead to exponential decay (with logarithmic corrections) of  $P(X, t)$ . This universal behavior also holds for short times, a fact that makes experimental observations readily achievable. Time permitting we then formulate the hitchhiker model where interacting molecules form aggregates, that lead to fluctuations in the diffusion field, and a many body mechanism for the exponential tails [2].

### References

- [1] E. Barkai and Stas Burov, Packets of diffusing particles exhibit universal exponential tails, Phys. Rev. Lett. **124**, 060603 (2020).
- [2] M. Hidalgo-Soria, and E. Barkai, The Hitchhiker model for Laplace diffusion processes in the cell environment, Phys. Rev. E **102**, 012109 (2020).

**Primary author:** BARKAI, Eli (Bar Ilan Univeristy)

**Presenter:** BARKAI, Eli (Bar Ilan Univeristy)

**Session Classification:** S2

Contribution ID: 50

Type: **30 minute lecture**

## Energy cascade in internal wave attractors

*Thursday, December 3, 2020 10:00 AM (30 minutes)*

Internal gravity waves play a primary role in geophysical fluids : they contribute significantly to mixing in the ocean and they redistribute energy and momentum in the middle atmosphere. In addition to their very interesting and very unusual theoretical properties, these waves are linked to one of the important questions in the dynamics of the oceans: the cascade of mechanical energy in the abyss and its contribution to mixing. Combining the physics of waves, dynamical systems theory and oceanography, I will discuss a unique self-consistent experimental and numerical setup that models a cascade of triadic interactions transferring energy from large-scale monochromatic input to multi-scale internal wave motion. I will also provide explicit evidence of a wave turbulence framework for internal waves.

**Primary author:** DAUXOIS, Thierry (CNRS & ENS de Lyon)

**Presenter:** DAUXOIS, Thierry (CNRS & ENS de Lyon)

**Session Classification:** S1

Contribution ID: 51

Type: **30 minute lecture**

## **Thermodynamics in biology: From molecular motors to metabolism**

*Friday, December 4, 2020 4:00 PM (30 minutes)*

I will describe recent progress in nonequilibrium thermodynamics based on stochastic thermodynamics and chemical reaction network theory. I will discuss the relevance of these results for biology and the many open challenges to be addressed.

**Primary author:** ESPOSITO, Massimiliano (University of Luxembourg)

**Presenter:** ESPOSITO, Massimiliano (University of Luxembourg)

**Session Classification:** S6

Contribution ID: 52

Type: **30 minute lecture**

## Using stochastic models to describe the coronavirus epidemic

*Thursday, December 3, 2020 9:30 AM (30 minutes)*

In December 2019, a novel new strain of coronavirus (COVID-19) was identified as it spread through China and subsequently throughout the world, resulting in a pandemic. As the health systems became overwhelmed, a need arose for real-time surveillance and modelling to identify the breaking points caused by increased numbers of infections and hospitalised individuals. We combined surveillance data for Scotland, detailing new COVID-19 cases, deaths, hospitalisations and critical care beds, with a modified stochastic Susceptible Exposed Infected Recovered Hospitalised Critical Dead (SEIR-HCD) model. The model parameters are adjusted daily, to fit the real-world data, using a Bayesian statistical particle filtering technique. The estimation technique uses an acceptance/rejection method combined with correlated multi-dimensional diffusion and drift model to effectively search the parameter space. We show close agreement between data and model output and discuss how changes in parameters reflect the changing transmission dynamics of the virus and severity of the disease.

**Primary authors:** Prof. KLECZKOWSKI, Adam (Univ. of Strathclyde); WELLS, Jonathan; Prof. ROBERTSON, Chris (Univ. of Strathclyde); Dr MARMARA, Vincent (University of Malta); YEUNG, Alan

**Presenter:** Prof. KLECZKOWSKI, Adam (Univ. of Strathclyde)

**Session Classification:** S1

Contribution ID: 53

Type: poster

## Detection of interaction and energy exchange with invisible partners in localized Brownian dumbbells

Thursday, December 3, 2020 6:00 PM (1 minute)

When recording trajectories of biomolecules in crowded media, a question of fundamental interest is whether a tracked molecule interacts with other molecules or structures invisible to the observer. One also wants to know whether energy exchange occurs during such interactions since out-of-equilibrium interactions can be a sign of a specific biological function. Addressing these questions using recorded single-particle trajectories is, in general, an ill-posed problem. In this work, we demonstrate how and when possible interactions and energy transfer between the particles can be detected in an idealized system consisting of two linked localized Brownian particles, where only one of the two trajectories is recorded.

To these means, we designed a Bayesian test for whether the observed trajectory corresponds to a single particle or 2 linked particles. The test leverages Bayesian statistics to compare the evidence for that the input trajectory's power spectrum is generated by an independent particle or a particle with a partner. Extensive numerical simulations allowed us to establish parameter regions, within which such partner detection is possible. As expected, the test is most sensitive to the link strength and the ratio of particle diffusivities. As a byproduct, we also obtained estimates of the localization strength and diffusivities of both particles.

For systems where a difference in diffusivities can be interpreted as a difference in local temperatures, we further extended our approach to determine whether the physical system is out of equilibrium. Using numerical simulations, we identified the parameter range where the distinction can be reliably made from recorded data.

Despite the simplicity of the model, the application of the method to real experimental trajectories may help identify the presence of an interaction partner, the interaction direction, and the presence of potential energy fluxes.

**Primary authors:** Dr SEROV, Alexander S. (Decision and Bayesian Computation, Department of Computational Biology, Department of Neurosciences, CNRS USR 3756, CNRS UMR 3571, Institut Pasteur, 25 rue du Docteur Roux, Paris, 75015, France); Dr VESTERGAARD, Christian L. (Decision and Bayesian Computation, Department of Computational Biology, Department of Neurosciences, CNRS USR 3756, CNRS UMR 3571, Institut Pasteur, 25 rue du Docteur Roux, Paris, 75015, France); Dr MASSON, Jean-Baptiste (Decision and Bayesian Computation, Department of Computational Biology, Department of Neurosciences, CNRS USR 3756, CNRS UMR 3571, Institut Pasteur, 25 rue du Docteur Roux, Paris, 75015, France)

**Presenter:** Dr SEROV, Alexander S. (Decision and Bayesian Computation, Department of Computational Biology, Department of Neurosciences, CNRS USR 3756, CNRS UMR 3571, Institut Pasteur, 25 rue du Docteur Roux, Paris, 75015, France)

**Session Classification:** Poster Session

Contribution ID: 54

Type: **poster**

## Finite element modelling of atomic force indentation of an animal cell

*Thursday, December 3, 2020 6:18 PM (1 minute)*

We present a model of atomic force microscope indentation measurements using the finite element method. The focus is set on a thorough representation of the complex structure of an animal cell. Crucial constituent is the cell cortex – a stiff layer of cytoplasmic proteins present on the inner side of the cell membrane. It plays a vital role in the mechanical interactions between cells. In our model, the cell cortex is modelled by a three-dimensional solid characterized primarily by its bending stiffness. This approach allows us to interpret the measurements of the mechanical properties of the cells, such as elasticity. During the simulations, we probe a broad range of parameters defining cell properties and experimental conditions. Finally, we derive a simple and closed-form formula that approximates the simulated results with satisfactory accuracy. Our formula is as easy to use as Hertz's function in order to extract cell properties from the measurement, with additional consideration of the cell inner structure.

**Primary authors:** KRZEMIEN, Leszek (Instytut Katalizy i Fizykochemii Powierzchni im. Jerzego Habera Polskiej Akademii Nauk); Ms GIERGIEL, Magdalena (Zakład Fizyki Nanostruktur i Nanotechnologii, Instytut Fizyki UJ); KUREK, Agnieszka (Jerzy Haber Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences); BARBASZ, Jakub (Instytut Katalizy i Fizykochemii Powierzchni im. Jerzego Habera PAN)

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

**Session Classification:** Poster Session

Contribution ID: 55

Type: **poster**

## Statistical physics of inhomogeneous transport equations: first passage to the space-dependent diffusion

*Thursday, December 3, 2020 6:01 PM (1 minute)*

As the science and modern technologies are seizing the realm of nanoscale systems, characterization of composite materials with solid-fluid and fluid-fluid interfaces has become a problem of broad interdisciplinary interest. Properties of such complex systems, which vary in space over microscopic scales, shape important processes in engineering and biology. Estimation of the inhomogeneous—space-dependent—transport coefficients that characterize these processes, e.g. the diffusion coefficient or the heat conductivity, is however a challenging task. Moreover, two alternative formulations of the inhomogeneous transport equations exist in the literature. Using the theory of statistical physics, in my talk I will show that the two formulations, often regarded as distinct models, are in fact equivalent. In particular, one of them conveniently links the mass diffusion equation with statistics of molecules' first-passage events, which provide an efficient inference technique for the space-dependent diffusion coefficient.

**Primary author:** Dr BELOUSOV, Roman (The Abdus Salam International Centre for Theoretical Physics)

**Co-authors:** Dr ROLDÁN, Edgar (The Abdus Salam International Centre for Theoretical Physics); Dr FRANKLIN MERGAREJO, Ricardo (The Abdus Salam International Centre for Theoretical Physics); Dr HASSANALI, Ali (The Abdus Salam International Centre for Theoretical Physics); Dr QAISRANI, Muhammad Nawaz (International School for Advanced Studies, The Abdus Salam International Centre for Theoretical Physics)

**Presenter:** Dr BELOUSOV, Roman (The Abdus Salam International Centre for Theoretical Physics)

**Session Classification:** Poster Session

Contribution ID: 57

Type: **not specified**

## Opening

*Thursday, December 3, 2020 8:50 AM (10 minutes)*

**Session Classification:** S1

Contribution ID: 58

Type: 20 minute talk

## Loopy Lévy flights enhance tracer diffusion in active suspensions

*Thursday, December 3, 2020 12:30 PM (20 minutes)*

Brownian motion is widely used as a model of diffusion in equilibrium media throughout the physical, chemical and biological sciences. However, many real-world systems are intrinsically out of equilibrium owing to energy-dissipating active processes underlying their mechanical and dynamical features. The diffusion process followed by a passive tracer in prototypical active media, such as suspensions of active colloids or swimming microorganisms, differs considerably from Brownian motion, as revealed by a greatly enhanced diffusion coefficient and non-Gaussian statistics of the tracer displacements. Although these characteristic features have been extensively observed experimentally, there is so far no comprehensive theory explaining how they emerge from the microscopic dynamics of the system. Here we develop a theoretical framework to model the hydrodynamic interactions between the tracer and the active swimmers, which shows that the tracer follows a non-Markovian coloured Poisson process that accounts for all empirical observations [1]. The theory predicts a long-lived Lévy flight regime of the loopy tracer motion with a non-monotonic crossover between two different power-law exponents. The duration of this regime can be tuned by the swimmer density, suggesting that the optimal foraging strategy of swimming microorganisms might depend crucially on their density in order to exploit the Lévy flights of nutrients. Our framework can be applied to address important theoretical questions, such as the thermodynamics of active systems, and practical ones, such as the interaction of swimming microorganisms with nutrients and other small particles (for example, degraded plastic) and the design of artificial nanoscale machines.

[1] K. Kanazawa, T. Sano, A. Cairoli, A. Baule; *Nature* 579, 364–367 (2020)

**Primary authors:** Dr KANAZAWA, Kiyoshi; Dr SANO, Tomohiko; Dr CAIROLI, Andrea; Dr BAULE, Adrian

**Presenter:** Dr BAULE, Adrian

**Session Classification:** S2

Contribution ID: 61

Type: **poster**

## Exploring shape space for densest random sequential adsorption packing

*Thursday, December 3, 2020 6:03 PM (1 minute)*

Random sequential adsorption of various shapes built of disks is studied to determine the shape, which follows to densest random packing. Using the evolutionary algorithm to sample the space of shapes, we found that independently of the number of used disks, the optimal shape tends to a triangle with rounded corners. Thus, we run the same algorithm to study packings built of rounded polygons. Both these approaches indicate that the shape building the densest RSA packings is the rounded triangle, for which the packing fraction is  $0.600608 \pm 0.000017$ , which is the highest known value so far.

**Primary authors:** Mr KOZUBEK, Konrad (Institute of Theoretical Physics, Jagiellonian University); CIEŚLA, Michał (Institute of Theoretical Physics, Jagiellonian University); Mr KUBALA, Piotr (Institute of Theoretical Physics, Jagiellonian University); Dr BAULE, Adrian (Queen Mary University of London)

**Presenter:** Mr KOZUBEK, Konrad (Institute of Theoretical Physics, Jagiellonian University)

**Session Classification:** Poster Session

Contribution ID: **62**

Type: **20 minute talk**

## **Pre-poster session**

*Thursday, December 3, 2020 5:40 PM (20 minutes)*

**Presenter:** GÓRA, Paweł (Jagiellonian University)

**Session Classification:** S3

Contribution ID: 63

Type: **poster**

## Force spectroscopy in the study of endometrial diseases

*Thursday, December 3, 2020 6:22 PM (1 minute)*

The endometrium is the tissue lining the uterus cavity. The most important role of this tissue is enabling the embryo to implant and providing it with good conditions for growth and development. According to many literature reports, cell and tissue mechanical properties have a significant role in many disease states. Changes in cell properties such as elasticity are observed in the case of various cancers or blood diseases.

The main technique for cell and tissue mechanical properties analysis is Force Spectroscopy. The force curves obtained during indentation reflect the interaction between the surface of the sample surface and the measuring probe. The course of these curves allows the determination of such properties as adhesion and Young modulus.

In this poster, we present results of research aimed at checking the relationship between Young's modulus of endometrial tissue and women's receptivity.

**Primary authors:** Mrs KUREK, Agnieszka (Jerzy Haber Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences); Dr BARBASZ, Jakub (Jerzy Haber Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences)

**Presenters:** Mrs KUREK, Agnieszka (Jerzy Haber Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences); Dr BARBASZ, Jakub (Jerzy Haber Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences)

**Session Classification:** Poster Session

Contribution ID: 64

Type: poster

## Moments of the Van Hove dynamic scattering law

*Thursday, December 3, 2020 6:23 PM (1 minute)*

Studying the dynamics of a system at the atomic level provides important information about the behaviour of the system. For example, studying the dynamics of enzymes allows us to understand their biological function. Among the available techniques, studying the dynamics of a system by means of neutron scattering is of exceptional meaning, as neutrons scatter at the nuclei themselves. Van Hove's functions  $G_s(r, t)$  and  $G_d(r, t)$ , as well its Fourier transforms  $I_s(k, t)$  and  $I_d(k, t)$  contain all accessible information on the dynamics of the system. In order to find the function  $I_s(k, t)$  for small times we use its lowest time derivatives taken at the time  $t = 0$ . These are also the moments of the scattering law  $S_s(k, \omega)$ . Moments of the odd orders are equal to zero, what results from the invariance of the mechanics equations with respect to the time inversion. We give even moments up to the tenth order.

**Primary author:** Dr WOJNAR, Ryszard (Instytut Podstawowych Problemów Techniki PAN)

**Presenter:** Dr WOJNAR, Ryszard (Instytut Podstawowych Problemów Techniki PAN)

**Session Classification:** Poster Session

Contribution ID: 65

Type: poster

## Generalised 'Arcsine' laws for run-and-tumble particle in one dimension

*Thursday, December 3, 2020 6:24 PM (1 minute)*

The 'Arcsine' laws of Brownian particles in one dimension describe distributions of three quantities: the time  $t_m$  to reach maximum position, the time  $t_r$  spent on the positive side and the time  $t_l$  of the last visit to the origin. Interestingly, the cumulative distribution of all three quantities are the same and given by Arcsine function. In this paper, we study distribution of these three times  $t_m$ ,  $t_r$  and  $t_l$  in the context of single run-and-tumble particle in one dimension, which is a simple non-Markovian process. We compute exact distributions of these three quantities for arbitrary time and find that all three distributions have a delta function part and a non-delta function part. Interestingly, we find that the distributions of  $t_m$  and  $t_r$  are identical (reminiscent of the Brownian particle case) when the initial velocities of the particle are chosen with equal probability. On the other hand, for  $t_l$ , only the non-delta function part is the same as the other two. In addition, we find explicit expressions of the joint distributions of the maximum displacement and the time at which this maxima occurs.

**Primary authors:** Mr SINGH, Prashant (ICTS-TIFR); Prof. KUNDU, Anupam (ICTS-TIFR)

**Presenter:** Mr SINGH, Prashant (ICTS-TIFR)

**Session Classification:** Poster Session

Contribution ID: 66

Type: **poster**

## Express your scientific track record in just three numbers

*Thursday, December 3, 2020 6:25 PM (1 minute)*

The growing popularity of bibliometric indexes goes hand in hand with their critique by those who claim that scientist's impact cannot be reduced to a single number. Some even believe that such a complex reality fails to submit to any quantitative description. We argue that neither of the two controversial extremes is true. With our new agent-based model ([doi.org/10.1073/pnas.2001064117](https://doi.org/10.1073/pnas.2001064117)) we can describe the emergence of citation curves very accurately.

In the model we assumed that some citations are distributed according to the rich get richer rule while some others are allocated totally at random. This yields a very accurate model that is governed by merely three easily interpretable parameters: productivity, total impact, and rho, which measures preferential vs. random rules ratio..

**Primary author:** Dr SIUDEM, Grzegorz (Warsaw University of Technology)

**Co-authors:** Mrs ŻOGAŁA-SIUDEM, Barbara (Systems Research Institute, Polish Academy of Sciences); Dr CENA, Anna (Warsaw University of Technology); Prof. GAGOLEWSKI, Marek (Deakin Universtiy)

**Presenter:** Dr SIUDEM, Grzegorz (Warsaw University of Technology)

**Session Classification:** Poster Session

Contribution ID: 68

Type: poster

## Nanoscale Lubrication in Model Biosystems as Rationalized in Terms of Fractons and Spectral-Mechanical Properties of Networked Biopolymers in Solutions

Thursday, December 3, 2020 6:26 PM (1 minute)

A concept of a biopolymer network immersed within an aqueous solution as addressed in terms of flexibility vs. mechanical stability criterion has been proposed. It is based on a transmission of correlated wave of (hydrogen) ions emerging from breaking in a massive way the hydrogen bonds between the biopolymers, such as hyaluronan, and their non-ideal aqueous solution's surroundings.

Based on the argumentation presented in a paper by Reuveni et al. [1] it has been demonstrated that there exists a clear connection between the  $\ln(N)$  (a natural logarithm of the biopolymer length  $N$ ) and an inverse of a difference between two major contributions of this Landau-Peierls instability type paradigm. Providing that the so-called Alexander-Orbach conjecture for the oscillating biopolymeric system applies [2,3] one of the contributions is of mechanical nature, with an exponent  $g$  represented by  $1/(2-3g)$  whereas the other appears to be a surface-to-volume characteristic exponent, attaining preferentially a value of ca.  $2/3$  for a three-dimensional adjacent (articulating) space.

It has been shown in a numerical way that for  $N$  of the order of million(s) biopolymer's residues, for example for hyaluronan equivalent to its molecular weight of  $10^6$ - $6 \times 10^6$  Daltons, a measure of the best viscoelastic efficiency for the hyaluronan, there exists an equality  $\ln(N) = b/[1/(2-3g) - 2/3]$  that, for example, for  $N=10^6$  gives the value of mechanical exponent  $g$  close to  $1/3$ , yielding according to [3,4], an excellent passage of the (hydrogen) ions' wave derived from a breakage of the adjacent hydrogen bonds in the biopolymer-solution system of interest, provided that the constant  $b$ , according to [1], can be taken at  $b=4.5$ . (In general, for the exponent  $g > 1/6$  holds.) The first results seem to be promising when thoroughly rationalizing nanoscale friction-lubrication properties of biopolymer-solution articulating/confined subspaces exposed to very small nano-Newton loading conditions. For another thermomechanical scenario describing phase-transition and relaxation kinetics of a biopolymeric system, see [5].

### References

- [1] S. Reuveni et al. PRL 100, 208101 (2008).
- [2] S. Alexander, R. Orbach J. Physique-LETTRES 43, L-625 (1982).
- [3] A. Gadomski et al. Tribol. Lett. 30, 83 (2008).
- [4] A. Gadomski et al. Mathematical Biosciences 244, 188 (2013) .
- [5] A. Gadomski, J. Łuczka, Acta Phys. Pol. B 28, 1827 (1997); A. Gadomski et al. Europ. Phys. J. B 91, 237 (2018).

Email address: agad@utp.edu.pl (to whom the correspondence can be addressed).

**Primary authors:** Dr BÉLDOWSKI, Piotr (Institute of Mathematics and Physics, Faculty of Chemical Technology and Engineering, UTP University of Science and Technology, Bydgoszcz, Poland); GADOMSKI, ADAM (UTP UNIVERSITY OF SCIENCE & TECHNOLOGY BYDGOSZCZ, POLAND)

**Presenter:** GADOMSKI, ADAM (UTP UNIVERSITY OF SCIENCE & TECHNOLOGY BYDGOSZCZ, POLAND)

**Session Classification:** Poster Session

Contribution ID: 69

Type: **poster**

## The effect of substrate roughness on random sequential adsorption packing properties

*Thursday, December 3, 2020 6:26 PM (1 minute)*

Adsorption on smooth and atomistically flat surface is well understood, while still very few works concern adsorption on rough and heterogeneous surfaces. In this study, we investigate the properties of packings of balls obtained via random sequential adsorption (RSA) on a sinusoidal substrate. Our main goal is to observe surface inhomogeneities on a scale smaller than particles' size. We study how various characteristics, such as packing fraction, packing growth kinetics, available surface function and 2-particle density correlation function depend on the wavenumber and the amplitude of a sine-wave-shaped surface. These quantities indeed allow us to discern very minute surface impurities from the packing alone.

**Primary author:** Mr KUBALA, Piotr (Institute of Theoretical Physics, Jagiellonian University)

**Co-author:** CIESLA, Michal (Institute of Theoretical Physics, Jagiellonian University)

**Presenter:** Mr KUBALA, Piotr (Institute of Theoretical Physics, Jagiellonian University)

**Session Classification:** Poster Session

Contribution ID: 71

Type: 20 minute talk

## Lévy Noise, Time-Reversal Symmetry, Nonequilibrium Stochastic Thermodynamics, and Bak's Sandpile

*Thursday, December 3, 2020 5:00 PM (20 minutes)*

The Brownian noise in nonequilibrium systems commonly contains more outliers. In that case the noise is best described with a Levy distribution. Many systems in which there are fluctuations around a steady-state throughput can be modeled as a Levy-noise-subjected particle in a parabolic potential. We consider an overdamped Brownian particle in a parabolic potential. If the noise is Levy, time-reversal symmetry for the particle's trajectory is violated. We formulate a parameter,  $r$ , to express and detect this violation. With solar flare data it is shown how  $r$  can be readily obtained and next used to obtain a good estimate of the stability index,  $\alpha$ , of the underlying noise. Self-organized-criticality, i.e. the famous avalanching sandpiles of Per Bak et al, can also be modeled with a Levy-noise-subjected particle on a potential. Preliminary results from such an approach are shown.

**Primary authors:** BIER, Martin (East Carolina University); YUVAN, Steven (East Carolina University)

**Presenter:** BIER, Martin (East Carolina University)

**Session Classification:** S3