34th M. Smoluchowski Symposium on Statistical Physics

Monday 27 September 2021 - Wednesday 29 September 2021

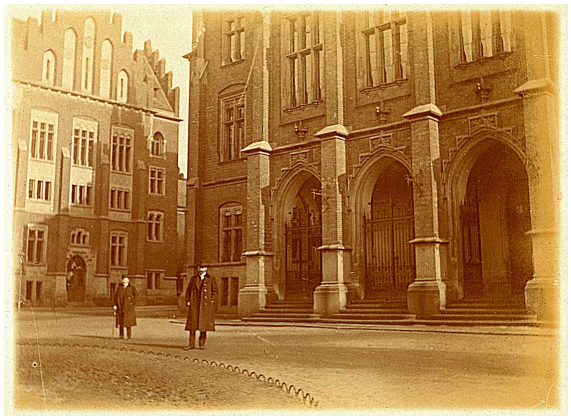
Online

Book of Abstracts

Contents

About

The Marian Smoluchowski Symposium on Statistical Physics is a cyclic scientific meeting organized annually in Poland since 1988. The conference is traditionally organized under the patronage of the Institute of Physics (now Institute of Theoretical Physics) and Mark Kac Center for Complex System Research at the Jagiellonian University in Kraków, and the consortium of other Polish academic institutions, i.e. the Institute of Chemical Physics, Polish Academy of Science (Warszawa), Silesian University of Technology (Gliwice), August Chełkowski Institue of Physics, Silesian University (Katowice) and Wrocław University of Technology. European Science Foundation was involved in the preparation and co-sponsoring of the symposium in the past within the program PESC/STOCHDYN and PESC/EPSD. In 2012 the conference has been organized and promoted with the assistance of the Division of Statistical and Nonlinear Physics (SNP), a part of the European Physical Society (EPS). Meeting in 2006 and in 2012 were organized under the patronage of the Polish Academy of Science and Arts and the Polish Academy of Science.



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Conference webpage: www.smoluchowski.if.uj.edu.pl

Conference platforms: MS Teams & Gather.town

Instructions for Participants

MS Teams

Invited Talk - 25 min. + 5 min. for discussion.

Contributed Talk - 15 min. + 5 min. for discussion.

Flash Talk - 5 min. (no discussion).

Recommended tutorials:

- https://www.youtube.com/watch?v=Yqxwc440GGM - Microsoft Teams - Conversations
- https://www.youtube.com/watch?v=DoJqHnpytUU - How to share your screen in a Microsoft Teams meeting

Strict timekeeping will be essential for the smooth running of the conference and we kindly ask for your cooperation.

All Presenters must be available on MS Teams at least 10 minutes before the start of their talks and are strongly encouraged to test their microphone, camera and presentation beforehand.

It is advised to prepare the presentation in PDF format.

Supported browsers: Microsoft Edge, Google Chrome, and Safari.

The desktop version is available.

Gather.town

IMPORTANT!: The following 2 items must be submitted to smoluchowski@uj.edu.pl by **Monday, September 27th (23:59 CEST)**. If you have any problems with formatting the required documents please do not hesitate to contact us for assistance.

Main document:

- .png or .jpg format are the only file types that may be used,
- Minimum width is 1000px (26.46cm),
- Minimum height is 600px (15.88cm),
- The maximum file size is 3 MB,
- No transparent background.

Preview “thumbnail” document:

- .png or .jpg format,
- A copy of the main poster document that has been made smaller,
- Recommended width is half of the main document,
- Recommended height is half of the main document.

During Poster Session

The Poster Session will take place in a specially designated virtual room, where posters will already be pre-loaded and organized in a grid similar to an in-person conference. Posters will be visible in the vicinity as "thumbnail" and upon interaction, the full-size poster will be accessible (details below).

Presenters: You should stand in the shaded square in front of your poster (marked by the respective number, see *List of Abstracts – Posters*). This shaded square is known as a “private space” and your audio/video will be shared with everyone solely within the range of this space. It will be also possible to use "blackboard" next to each poster and share the screen within/outside the "private space".

All Participants: To interact with a poster, Participants will walk up to the poster and press the “x” key to enter a full-screen viewing.

IMPORTANT!: The link to access the Poster Session will be provided on the MS Teams and sent *via* e-mail on **Monday, September 27th**. In the meantime, (i.e. between the Sessions and before the commencement of the Poster Session) Participants are highly encouraged to freely explore the Symposium virtual space. In the case of any inquires regarding the Gather.town please contact the on-site Admin, who will be present at the Symposium virtual space.

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Recommended tutorials:

- https://support.gather.town/help/movement-and-basics,
- https://support.gather.town/help/browser-settings-and-permissions.

Supported browsers: Google Chrome, Mozilla Firefox, and Safari (beta).

The desktop version is available.

Timetable

Symposium will take place according to
Central European Summer Time (CEST/UTC+2:00/GMT+2:00)

IT: Invited Talk CT: Contributed Talk FT: Flash Talk

Monday, 27/09

8:45–9:00		**Opening Ceremony**	
Session 1		*Chair: Ewa Gudowska-Nowak*	
9:00–9:30	IT	**Somrita Ray**	Stochastic resetting: When does it accelerate diffusive transport?
9:30–10:00	IT	**Trifce Sandev**	Resetting dynamics and random search in heterogeneous media
10:00–10:20	CT	**Prashant Singh**	Extremal statistics for stochastic resetting systems
10:20–10:40	CT	**RK Singh**	Backbone diffusion and first-passage dynamics in a comb structure with confining branches under stochastic resetting
10:40–11:00	CT	**Ofir Tal-Friedman**	Experimental realization of diffusion with stochastic resetting
11:00–12:00		**Break**	
Session 2		*Chair: Michał Cieśla*	
12:00–12:30	IT	**Yuri Tarasevich**	Nano-wire based transparent electrodes: a mean-field approach
12:30–12:50	CT	**Paweł Karbowniczek**	Investigation of ring and star-shaped polymers in confined geometries
12:50–13:10	CT	**Reimer Kühn**	The Fate of Articulation Points and Bredges in Percolation
13:10–13:30	CT	**Nikolai Lebovka**	Relaxation of random sequential adsorption packings of discorectangles aligned on a line
13:30–13:50	CT	**Anna Danilova**	Network analysis of the novel "The Master and Margarita" by M. A. Bulgakov

13:50–13:55	FT	**Michał Łepek**	Combinatorial approach to modeling coagulation phenomena
13:55–14:00	FT	**Andrei Eserkepov**	Exact percolation probabilities on plane, cylinder, and torus: site percolation on a square lattice
14:00–16:00		**Break**	
Session 3		*Chair: Nikolai Lebovka*	
16:00–16:30	IT	**Salvatore Torquato**	Disordered Hyperuniform Particle Packings
16:30–16:50	CT	**Piotr Kubala**	Liquid crystal phases of banana-shaped hard-core molecules composed of balls
16:50–17:10	CT	**Robert M. Ziff**	Percolation on non-planar lattices
17:10–17:30	CT	**Konrad Kozubek**	Exploring 2D shape space: the hunt for the densest RSA packings
17:30–17:50	CT	**Luca Petrone**	Random Sequential Adsorption of Oriented Rectangles with Random Aspect Ratio
17:50–17:55	FT	**Agnieszka Chrzanowska**	Diffusion of nickel atoms into silver regimes in layered nanostructures-molecular dynamics simulations
17:55–18:00	FT	**Prasad V V**	Asymptotic tails of 2D Driven Granular Gases

Symposium will take place according to
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IT: Invited Talk CT: Contributed Talk FT: Flash Talk

Tuesday, 28/09

Session 4		*Chair: Trifce Sandev*	
9:00–9:30	IT	**Alberto Imparato**	Critical behaviour of interacting thermodynamic machines
9:30–9:50	CT	**Ohad Shpielberg**	Thermodynamic uncertainty relations for many-body systems with fast jump rates and large occupancies
9:50–10:10	CT	**Krzysztof Ptaszyński**	Non-Markovianity boosting the performance of a quantum Otto engine
10:10–10:30	CT	**Salambô Dago**	Fast is hot: energetics of information erasure and the overhead to Landauer's bound
10:30–10:50	CT	**Katarzyna Sznajd-Weron**	"Private Truths, Public Lies" within agent-based modeling
10:50–10:55	FT	**Seyed Mohsen Jebreiil Khadem**	Stochastic thermodynamics of anomalous diffusion generated by scaled and fractional Brownian motions
10:55–11:00	FT	**Andrzej Krawiecki**	The q-neighbor Ising model on multiplex networks with partial overlap
11:00–12:00		**Break**	
Session 5		*Chair: Jakub Barbasz*	
12:00–12:30	IT	**Maciej Lisicki**	Elastohydrodynamics of microscale swimming
12:30–12:50	CT	**Denis Grebenkov**	Paradigm shift in diffusion-mediated surface phenomena
12:50–13:10	CT	**Katarzyna Górska**	Integral decomposition for the solutions of the generalized Cattaneo equation

13:10–13:30	CT	**Serg Pozdneev**	Resonances in Electron Scattering by Molecules
13:30–13:35	FT	**Michał Bogdan**	Stochastic jetting and dripping in confined soft granular flows
13:35–13:40	FT	**Kasper Meerts**	Diffraction and interference with run-and-tumble particles
14:00–16:00		**Break**	
Session 6		*Chair: Katarzyna Górska*	
16:00–16:30	IT	**Paul Bressloff**	Accumulation time of stochastic processes with resetting
16:30–16:50	CT	**Viktor Stojkoski**	Geometric Brownian Motion under Stochastic Resetting: A Stationary yet Non-ergodic Process
16:50–17:10	CT	**Marcus Dahlenburg**	Random amplitude stochastic resetting
17:10–17:30	CT	**Aleksander Stanislavsky**	The role of the Laplace distribution in stochastic resetting
17:30–17:50	CT	**Dante R. Chialvo**	Gut's complexity
17:50–17:55	FT	**Ofek Lauber**	First passage under restart for discrete space and time
17:55–18:00	FT	**Seongyu Park**	Bayesian inference of Lévy walks via hidden Markov models: parameter estimation and model classification
18:00–19:00		**Poster Session on Gather.town**	

Symposium will take place according to
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IT: Invited Talk CT: Contributed Talk FT: Flash Talk

Wednesday, 29/09

Session 7		*Chair: Katarzyna Sznajd-Weron*	
9:00–9:30	IT	**Ralf Metzler**	Non-Gaussian statistics in soft & bio-matter
9:30–09:50	CT	**Yuval Scher**	Unified Approach to Gated Reactions on Networks
09:50–10:10	CT	**Oleksandr Kliushnichenko**	Epidemic-Driven Collapse in a System with Limited Economic Resource
10:10–10:30	CT	**Tal Agranov**	Extinctions of coupled populations, and rare event dynamics under non-Gaussian noise
10:30–10:50	CT	**Maciej Majka**	The mechanics of domain formation in the gene expression profiles
10:50–10:55	FT	**Richard Ho**	Achieving robustness and precision in the developing spinal cord with system-level feedback
10:55–11:00	FT	**Ryszard Wojnar**	Collagen as Hopf's fibration
11:00–12:00		**Break**	
Session 8		*Chair: Ralf Metzler*	
12:00–12:30	IT	**Emmanuel Trizac**	Enhancing transport by shaping barriers (beating activation energies)
12:30–13:00	IT	**Jakub Spiechowicz**	Colossal Brownian, yet non-Gaussian diffusion in a periodic potential
13:00–13:20	CT	**Martin Evans**	Interacting Persistent Random Walkers
13:20–13:40	CT	**Gianni Pagnini**	Should I stay or should I go? Zero-size jumps in random walks for Lévy flights
13:40–14:00	CT	**Karol Capała**	Inertial Lévy flights in bounded domains

14:00–16:00		**Break**	
Session 9		*Chair: Paweł F. Góra*	
16:00–16:30	IT	**Tomás S. Grigera**	Dynamic crossover in homogeneous active matter
16:30–16:50	CT	**Igor Sokolov**	Brownian yet non-Gaussian diffusion in models of disordered systems
16:50–17:10	CT	**Monika Muszkieta**	Simulation and tracking of fractional particles motion. From microscopy video to statistical analysis. A Brownian bridge approach
17:10–17:30	CT	**Yann Lanoiselée**	Detecting Transient Trapping from a Single Trajectory: A Structural Approach
17:30–17:50	CT	**Teodor Buchner**	How fast is the ECG signal and why do we need a kinetic theory of conductance
17:50–17:55	FT	**Samudrajit Thapa**	Leveraging large deviation statistics to decipher the stochastic properties of measured trajectories
17:55–18:00	FT	**Jarosław Klamut**	The crucial role of inter-trade times in volatility clustering: a continuous-time random walk description
18:00–18:10		**Closing Ceremony**	

List of Abstracts – Talks

Symposium will take place according to
Central European Summer Time (CEST/UTC+2:00/GMT+2:00)

Session 1

Monday 27/09, 9:00 – 9:30

Stochastic resetting: When does it accelerate diffusive transport?

Somrita Ray IT

Department of Chemistry, Indian Institute of Technology Tirupati

Stochastic resetting [1] can either accelerate or delay a dynamical process that takes a random time to complete (i.e., a first-passage process). Tuning system parameters can invert the effect of resetting on the mean completion time of the process, leading to a *resetting transition*. In this talk, I shall first explore the exact conditions where stochastic resetting accelerates diffusive transport for a couple of analytically tractable systems, viz.,

(i) diffusion in a linear potential, where the resetting transition is found to be governed by the Péclet number [2],

(ii) diffusion in a logarithmic potential, that exhibits a series of dynamical transitions when the constant strength of the potential in the units of thermal energy, is tuned [3].

Based on the common trends that these model systems show, a general framework can be proposed that reveals that the resetting transition is governed by an interplay between thermal and potential energy; when thermal energy dominates the dynamics, resetting can expedite the process [4]. Finally, considering a toy model for space-dependent diffusion, I shall show that whenever a dynamical process is diffusion-controlled, resetting can, in principle, accelerate it [5]. We believe that our analysis will be useful in a variety of natural as well as man-made systems where resetting plays a crucial role in diffusive transport.

References:

[1] M. R. Evans, S. N. Majumdar, and G. Schehr, J. Phys. A: Math. Theor. 53, 193001 (2020).
[2] S. Ray, D. Mondal and S. Reuveni, J. Phys. A: Math. Theor. 52, 255002 (2019).
[3] S. Ray and S. Reuveni, J. Chem. Phys. 152, 234110, (2020).
[4] S. Ray and S. Reuveni, J. Chem. Phys. (Comm.) 154, 171103, (2021).
[5] S. Ray, J. Chem. Phys. 153, 234904, (2020).

Monday 27/09, 9:30 – 10:00

Resetting dynamics and random search in heterogeneous media

Trifce Sandev IT

Macedonian Academy of Sciences and Arts, Skopje, Macedonia

Theoretical investigation of diffusion in heterogeneous media (such as materials with impurities, defects, fractal and random heterogeneous structures and combs, crowded environments, etc.) currently receives a considerable interest. The corresponding heterogeneous diffusion process often becomes anomalous due to the geometric constraints, random potential effects or variations of the local diffusion coefficients in the heterogeneous media. We will present results for the first passage and first hitting times for different random search processes in such complex environment. Introduction of a stochastic resetting in the corresponding heterogeneous diffusion process leads to a non-trivial transition of the system to a nonequilibrium stationary state. We will quantify the transition to the stationary state in terms of a large deviation function, which defines the separation of the region in which relaxation to the nonequilibrium stationary state has been achieved from the region in which the system is still in a transient state. We will also show that the heterogeneous diffusion process might be closely related to the turbulent diffusion represented by the inhomogeneous advection-diffusion equation, and the (generalized) geometric Brownian motion used to model stock prices.

Monday 27/09, 10:00 – 10:20

Extremal statistics for stochastic resetting systems

Prashant Singh [1] and Arnab Pal [2]

CT

[1] *ICTS-TIFR*

[2] *IIT, Kanpur, India*

While averages and typical fluctuations often play a major role in understanding the behavior of a nonequilibrium system, this nonetheless is not always true. Rare events and large fluctuations are also pivotal when a thorough analysis of the system is being done. In this context, the statistics of extreme fluctuations in contrast to the average plays an important role, as has been discussed in fields ranging from statistical and mathematical physics to climate, finance, and ecology. Herein, we study extreme value statistics (EVS) of stochastic resetting systems, which have recently gained significant interest due to its ubiquitous and enriching applications in physics, chemistry, queuing theory, search processes, and computer science. We present a detailed analysis for the finite and large time statistics of extremals (maximum and arg-maximum, i.e., the time when the maximum is reached) of the spatial displacement in such system. In particular, we derive an exact renewal formula that relates the joint distribution of maximum and arg-maximum of the reset process to the statistical measures of the underlying process. Benchmarking our results for the maximum of a reset trajectory that pertain to the Gumbel class for large sample size, we show that the arg-maximum density attains a uniform distribution independent of the underlying process at a large observation time. The results are augmented with a wide spectrum of Markov and non-Markov stochastic processes under resetting, namely, simple diffusion, diffusion with drift, Ornstein-Uhlenbeck process, and random acceleration process in one dimension. Rigorous results are presented for the first two setups, while the latter two are supported with heuristic and numerical analysis.

Monday 27/09, 10:20 – 10:40

Backbone diffusion and first-passage dynamics in a comb structure with confining branches under stochastic resetting

RK Singh [1], Trifce Sandev, Alexander Iomin and Ralf Metzler

CT

[1] *RKMVERI- Belur Math, Howrah, India*

[2] *Macedonian Academy of Sciences and Arts, Skopje, Macedonia*

[3] *Department of Physics, Technion*

[4] *University of Potsdam*

We study the diffusive motion of a test particle in a two-dimensional comb structure consisting of a main backbone channel with continuously distributed side branches, in the presence of stochastic Markovian resetting to the initial position of the particle. We assume that the motion along the infinitely long branches is biased by a confining potential. The crossover to the steady state is quantified in terms of a large deviation function, which is derived for the first time for comb structures in present paper. We show that the relaxation region is demarcated by a nonlinear “light-cone” beyond which the system is evolving in time. We also investigate the first-passage times along the backbone and calculate the mean first-passage time and optimal resetting rate.

Monday 27/09, 10:40 – 11:00

Experimental realization of diffusion with stochastic resetting

Ofir Tal-Friedman [1], Arnab Pal [2], Amandeep Sekhon [1], Shlomi Reuveni [1] and Yael Roichman [1]

CT

[1] *Tel Aviv University*

[2] *Indian Institute of Technology Kanpur*

Stochastic resetting is prevalent in natural and man-made systems, giving rise to a long series of nonequilibrium phenomena. Diffusion with stochastic resetting serves as a paradigmatic model to study these phenomena but lacked a well-controlled platform by which it can be studied experimentally. Here, we report the experimental realization of colloid diffusion and resetting via holographic optical tweezers. We provide the first experimental corroboration of theoretical results and measure the energetic cost of resetting in steady-state and first-passage scenarios. In both cases, we show that this cost cannot be made arbitrarily small because of fundamental constraints on realistic resetting protocols.

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Session 2

Monday 27/09, 12:00 – 12:30

Nano-wire based transparent electrodes: a mean-field approach

Yuri Tarasevich [1], Irina Vodolazskaya [1] and Andrei Eserkepov [1]

IT

[1] *Astrakhan State University*

Transparent electrodes are important components of modern optoelectronic devices such as touch-screens, heaters, and solar cells. One of the most widely used kinds of transparent electrode consists of a transparent, poorly conductive film containing randomly distributed highly conductive fillers such as nanowires, nanotubes, nanorods, and nanorings.

Using a mean-field approach, we evaluate the electrical conductivity of two-dimensional systems with rodlike and ringlike conductive fillers (wires). The concentration of fillers is supposed to be significantly higher than the percolation threshold. Instead of considering a random resistor network produced by all conductive fillers, we study one filler in the mean field generated by all other conductive fillers. Three limiting cases are of our specific interest, i.e., wire-resistance dominated regime, junction-resistance dominated regime, and equal wire and junction resistances.

We compare the electrical conductivity obtained within our mean-field approximation with the results of direct computations of the underlying random resistor networks as well with the analytical evaluations of other authors [1,2].

1. Kumar, N. S. Vidhyadhiraja, and G. U. Kulkarni, Current distribution in conducting nanowire networks, J. Appl. Phys. 122, 045101 (2017).

2. C. Forró, L. Demkó, S. Weydert, J. Vöoröos, and K. Tybrandt, Predictive model for the electrical transport within nanowire networks, ACS Nano 12, 11080–11087 (2018).

Monday 27/09, 12:30 – 12:50

Investigation of ring and star-shaped polymers in confined geometries

Paweł Karbowniczek [1], Joanna Hałun [2], Piotr Kuterba [3] and Zoriana Danel [1]

CT

[1] *Faculty of Materials Engineering and Physics, Cracow University of Technology, Poland*

[2] *Institute of Nuclear Physics, Polish Academy of Sciences, Poland*

[3] *Faculty of Physics, Astronomy and Applied Computer Sciences, Jagiellonian University in Cracow, Poland*

We investigate the dimensionless layer monomer density profiles of a dilute solution of ideal ring and star polymers confined in a slit geometry of two walls. We analyzed cases with both attractive and repulsive walls as well as one attractive and one repulsive wall. Additionally, we performed molecular dynamics simulations of a dilute solution of ring and star-shaped polymers. Analytical and numerical results were compared with the case of linear polymers. The obtained results indicate that ring and star-shaped polymers can be used for the production of new functional materials, because properties of their solutions depend on their topology and the nature of surfaces that confine them.

J. Hałun, P. Karbowniczek, P. Kuterba, and Z. Danel, Investigation of Ring and Star Polymers in Confined Geometries: Theory and Simulations, Entropy 23, 242 (2021)

Monday 27/09, 12:50 – 13:10

The Fate of Articulation Points and Bredges in Percolation

Reimer Kühn [1], Haggai Bonneau [2], Ido Ishby [2], Ofer Biham [2] and Eytan Katzav [2] CT

[1] *King's College London*

[2] *Hebrew University, Jerusalem*

Articulation points (APs) are *nodes* in complex networks whose removal would break the network component on which they are located into two or more disconnected components, while bredges (bridge-edges) are *edges* whose removal would break the network component on which they are located into two components. APs and bredges are thus crucial for the integrity and functionality of complex networks. In this talk we investigate the statistics of articulation points and bredges in complex networks in which bonds are randomly removed in a percolation process. Because of the heterogeneous nature of complex networks, the probability of a node to be an articulation point, or of an edge to be a bredge will not be homogeneous across the network. We therefore analyze full distributions of articulation point probabilities as well as bredge probabilities, using a message-passing approach to the problem, both for large single instances, and for networks in the configuration model class in the thermodynamic limit. We reveal, and are able to rationalize, a significant amount of structure in the evolution of articulation point and bredge probabilities in response to random bond removal. We argue that our results could be exploited in a variety of applications, including approaches to network dismantling or to vaccination and islanding strategies to prevent the spread of epidemics or of blackouts in process networks. Further details in Phys.Rev. E **103**, 042302 (2021).

Monday 27/09, 13:10 – 13:30

Relaxation of random sequential adsorption packings of discorectangles aligned on a line

Nikolai Lebovka [1], Mykhailo Tatochenko [1], Nikolai Vygornitskii [1] and Yuri Tarasevich [2] CT

[1] *Laboratory of Physical Chemistry of Disperse Minerals, F. D. Ovcharenko Institute of Biocolloidal Chemistry, NAS of Ukraine*

[2] *Laboratory of Mathematical Modeling, Astrakhan State University*

Relaxation of packing of elongated particles (discorectangles) aligned on a line was studied numerically. The aspect ratio (length-to-width ratio) for the discorectangles was varied within the range $\varepsilon \in [1; 50]$. The initial jamming (saturated) state was produced using the basic variant of the random sequential adsorption (RSA) model with random positions and orientations of particles. The relaxation was done accounting for the rotational and translational diffusion motions of particles with their centers located on a line. Effects of aspect ratio ε on kinetics of relaxation, orientation order parameter and distribution function of the distances between nearest-neighbor discorectangles were analized. The transport properties of the obtained 1d systems were also analyzed using the diffusion of a tracer particle (random walker) between the nearest-neighbor discorectangles. In the relaxed states the anomalous diffusion was observed with hopping exponent $d_w > 2$ dependent upon ε.

Monday 27/09, 13:30 – 13:50

Network analysis of the novel "The Master and Margarita" by M. A. Bulgakov

Anna Danilova [1] and Yuri Tarasevich [1]

CT

[1] *Astrakhan State University*

The network analysis of the structure of social relations in one of the most popular novels in Russian of the Soviet era by M. A. Bulgakov “The Master and Margarita” was carried out. The structure of the novel is complex, i.e., there is novel in novel. In our study, only relations between explicitly present and acting characters were taken into account; the characters mentioned and expected connections were not taken into consideration. Based on the character interaction matrix, a graph was constructed, the vertices of which are the characters of the novel, while the edges correspond to relation between them. In our study, only the explicit interaction of the characters on the stage was considered. Interaction, i.e., bidirectional action, leads to the fact that, in our study, the social network is described by an ordinary, rather than directed graph. The largest connected component of the graph consists of 153 characters.

Degree, betweenness, closeness, eigenvector, assortativity coefficient were computed to characterize the network.

The assortativity coefficient of the network under consideration equals to -0.177, which indicates artificiality of the network. The structure of communities in the network was analyzed using the Girvan—Newman algorithm. In addition to the obvious large communities — the characters from the Gospel part of the novel, the characters of the Moscow part of the novel, the characters of the other world — the algorithm also revealed a more subtle structure in the Moscow part of the novel: communities of writers, a hospital, and a theater. Using the analysis of centralities, a group of main characters has been detected. It turned out unexpectedly that in the Gospel part of the novel, the central character is Afranius, rather than Pontius Pilate.

Monday 27/09, 13:50 – 13:55

Combinatorial approach to modeling coagulation phenomena

Michał Łepek FT

Warsaw University of Technology, Faculty of Physics

Coagulation (aggregation) is a phenomenon that consists of combining clusters into larger clusters, with the probability of merging depending on the size (or mass) of these clusters. Such an abstract definition causes that we can find coagulation in a great number of real processes: starting from blood coagulation, through the processes known from food and polymer processing, to the creation of protoplanetary disks (accretion). Several theoretical approaches to the coagulation processes have been proposed over the years. The best-known analytical approach is one based on the Smoluchowski equation [1]. In the presentation, we will briefly discuss solutions that arise from the Smoluchowski equation and present other theoretical approaches (stochastic and combinatorial). The latter,i.e. the combinatorial approach, can be seen as a novelty in the field [2]. We will discuss in detail its requirements and solutions that were recently obtained (e.g., solution for the electrorheological coagulation [3]). These theoretical results were tested against numerical simulations and proved their high accuracy. The current status of the knowledge and open problems in the filed will be presented.

References

[1] P.L. Krapivsky, S. Redner and E. Ben-Naim: A Kinetic View of Statistical Physics (Chapter5), Cambridge University Press, New York 2010.
[2] M. Łepek, A. Fronczak, P. Fronczak: Rep.Math.Phys.88(1), 89-113 (2021), Coalescense with arbitrary-parameter kernels and monodisperse initial conditions: A study within combinatorial framework.
[3] M. Łepek, A. Fronczak, P. Fronczak: Phys.D 415,132756 (2021), Combinatorial solutions to coagulation kernel for linear chains.

Monday 27/09, 13:55 – 14:00

Exact percolation probabilities on plane, cylinder, and torus: site percolation on a square lattice

Andrei Eserkepov [1], Renat Akhunzhanov [1] and Yuri Tarasevich [1]

FT

[1] *Astrakhan State University*

For site percolation on a square lattice, exact percolation probabilities on plane, cylinder, and torus has been found. Topological dynamic programming was applied to improve performance. Topologically equivalent states of the system and their horizontal reflections were combined. In the case of a torus and a cylinder, the shifts of topological states were also taken into account. Percolation probabilities were obtained for systems up to size $L = 16$ (square), up to $L = 17$ (cylinder), up to $L = 9$ (torus). Along with a finite size scaling analysis, percolation probabilities provide an efficient method to obtain the percolation threshold.

Symposium will take place according to
Central European Summer Time (CEST/UTC+2:00/GMT+2:00)

Session 3

Monday 27/09, 16:00 – 16:30

Disordered Hyperuniform Particle Packings

Salvatore Torquato IT

Princeton University

The study of hyperuniform states of matter is an emerging multidisciplinary field, influencing and linking developments across the physical sciences, mathematics and biology [1,2]. A hyperuniform many-particle system in d-dimensional Euclidean space is characterized by an anomalous suppression of large-scale density fluctuations relative to those in typical disordered systems, such as liquids and amorphous solids. As such, the hyperuniformity concept generalizes the traditional notion of long-range order to include not only all perfect crystals and quasicrystals, but also exotic disordered states of matter. Disordered hyperuniform states have attracted great attention across many fields over the last two decades because they can have the character of crystals on large length scales but are isotropic like liquids. This hybrid crystal-liquid attribute endows them with unique or nearly optimal, direction-independent physical properties and robustness against defects. I will briefly review the hyperuniformity concept and then discuss a variety of different disordered article packings that are hyperuniform [1,2,3].

1. S. Torquato and F. H. Stillinger, “Local Density Fluctuations, Hyperuniform Systems, and Order Metrics,” Phys. Rev. E, 68, 041113 (2003).

2. S. Torquato, “Hyperuniform States of Matter,” Phys. Reports, 745, 1 (2018).

3. S. Torquato, Perspective: “Basic Understanding of Condensed Phases of Matter via Packing Models,” J. Chem. Phys. 149, 020901 (2018).

Monday 27/09, 16:30 – 16:50

Liquid crystal phases of banana-shaped hard-core molecules composed of balls

Piotr Kubala [1], Wojciech Tomczyk [1] and Michał Cieśla [1]

CT

[1] *Institute of Theoretical Physics, Jagiellonian University, Kraków, Poland*

Liquid crystals are a state of matter with the properties of both liquids and solids. They have a long research history dating back to the 19th century and have found countless applications, with LCDs being arguably the most important one of them. As demonstrated by Onsager, the phase transition between isotropic liquid and nematic liquid crystal can be induced by excluded volume effects within the hard spherocylinder model. It turns out that other hard-core particle systems exhibit a variety of different liquid crystal phases. We have performed molecular dynamic Monte Carlo simulations of achiral banana-shaped particles built from hard spheres in the NpT ensemble with varying bend angle and particles density. We have identified four distinct liquid crystal phases. The most notable one is twist-bend nematic, where the preferred direction varies in space with a periodic, heliconical pattern, displaying a broken chiral symmetry.

Monday 27/09, 16:50 – 17:10

Percolation on non-planar lattices

Robert M. Ziff

CT

Center for the Study of Complex Systems, and Department of Chemical Engineering

Percolation on non-planar lattices, such as lattices with crossing bonds, are generally expected to be in the two-dimensional universality class of ordinary percolation, and indeed that is the case for the leading behavior. However, we have found that the corrections to scaling, as characterized by the exponent Omega, are different for the non-planar system. This might imply that the usual corrections exponent is zero here due to some symmetry of the system. For a non-planar system, we consider bond percolation on the square covering lattice, which is equivalent to site percolation on the bond covering lattice. We also can consider a multilayer square lattice as an example of a non-planar system. We discuss methods to determine the threshold and the corrections exponent accurately.

Monday 27/09, 17:10 – 17:30

Exploring 2D shape space: the hunt for the densest RSA packings

Konrad Kozubek [1], Piotr Kubala [1], Michał Cieśla [1] and Adrian Baule [2]

[1] *Institute of Theoretical Physics, Jagiellonian University, Kraków, Poland*

[2] *Queen Mary University of London*

Random sequential adsorption (RSA) of various polydisks and rounded polygons is studied to determine the shape, which forms the densest packings. Covariance matrix adaptation evolution strategy (CMA-ES), an evolutionary optimization algorithm is used to search for optimal shapes. We found that independently of the number of component disks, the optimal polydisk resembles a triangle with rounded corners. Therefore we also explored variously parametrized spaces of rounded polygons using the same approach. All carried out optimizations indicate that the shape building the densest RSA packings is the rounded triangle for which the packing fraction is 0.600608 ± 0.000017, which is the highest known value so far. Properties of the triangle's contact function can be used to illustrate why this shape is capable of forming dense RSA packings.

Monday 27/09, 17:30 – 17:50

Random Sequential Adsorption of Oriented Rectangles with Random Aspect Ratio

Luca Petrone and Michał Cieśla [1]

CT

[1] *Institute of Theoretical Physics, Jagiellonian University, Kraków, Poland*

Random Sequential Adsorption is a very simple protocol that generates random loose packings. It takes a virtual particle, randomly chooses its position and orientation, and then checks if it does not overlap with any object already placed in the packing. If so, the virtual particle is added, otherwise it is removed.

Typically, the shape that is to be deposited is always the same. In this study, instead, we have studied a RSA of oriented rectangles of fixed area but random side length ratio.

The calculated packing density at saturation (0.678689) is considerably higher than any other else RSA.

Also, this value is dependent on the random distribution that is used to select the aspect ratio. A power-law

$$p_f(x) = (\alpha + 1)x^{\alpha}$$

was considered. The density at saturation is increasing with α and the limit $\alpha \to \infty$ was estimated.

Monday 27/09, 17:50 – 17:55

Diffusion of nickel atoms into silver regimes in layered nanostructures - molecular dynamics simulations

Agnieszka Chrzanowska FT

Department of Physics, Kraków University of Technology, ul. Podchorążych 1, 30-084 Kraków, Poland

Silver and nickel composites are peculiar for many reasons. As pure, both of these metals exhibit fcc crystal structures, but their lattice constants are much different. Because in the solid state they are almost insoluble, in the case of flat surfaces it may result in occurring of superlattice arrangement resulting from the mistmatch of lattice constants, with silver atoms well separated from nickel atoms. When temperature is raised the situation changes. If only one silver nanolayer deposited on the nickel layer is heated, it disappears through the desorption mechanism. However, if a silver nanolayer is confined between two nickel layers, desorption mechanism is no longer possible. Now, since melting temperatures of nickel and silver are also very different, an interesting case to study occurs, when one nanolayer is solid and the other is liquid. Taking also into account that nanoparticles are already known to exhibit lowered temperature of melting, one expects that this phenomenon will occur also in the case of nanolayers. In the presentation we will show the results obtained from the molecular dynamics where a multilayered silver-nickel structure undergoes heating and cooling. Especially interesting result has been obtained for a structure that was very slowly cooled down from a completely liquid state. One observes here nickel atoms diffusing into silver regime and creation of the alloy nanolayer in coexistence at the same time with pure nickel layers. Such an effect – possibility to change silver nanolayer onto silver-nickel alloy nanolayer upon confinement at increased temperature has not been previously discussed. Other observed tendencies are also presented.

Monday 27/09, 17:55 – 18:00

Asymptotic tails of 2D Driven Granular Gases

Prasad V V [1], R Rajesh [1], Dibyendu Das [1] and Sanjib Sabhapandit [1]

FT

[1] *Cochin University of Science and Technology*

The granular gas is a paradigm for understanding the effects of inelastic interactions in granular materials. Through this work, we obtain analytical results for a microscopic model for a granular gas where particles with two-dimensional velocities are driven homogeneously and isotropically by reducing the velocities by a factor and adding a stochastic noise. We find two universal regimes. For generic physically relevant driving, we find that the tail of the velocity distribution is a Gaussian with additional logarithmic corrections. Thus, the velocity distribution decays faster than the corresponding equilibrium gas. The second universal regime is less generic and corresponds to the scenario described by kinetic theory. Here, the velocity distribution is shown to decays an exponential with additional logarithmic corrections. The universality in the statistics is solely depends on the inelastic collisional interaction, and the presence of steady state. Therefore one would expect this to be valid for a large range of system parameters and for experimental scenarios of driven granular systems.

Symposium will take place according to
Central European Summer Time (CEST/UTC+2:00/GMT+2:00)

Session 4

Tuesday 28/09, 09:00 – 09:30

Critical behaviour of interacting thermodynamic machines

Alberto Imparato IT

Department of Physics and Astronomy, Aarhus University

It is known that in an equilibrium system approaching a critical point, the response to a change in an external thermodynamic force can become significantly large.

In other words, an equilibrium system at the verge of a second-order phase transition is highly susceptible to external thermodynamic forces.

Starting from this premise, in my talk I will discuss the properties of systems of interacting thermodynamic machines that operate at the verge of a phase transition.

I will focus on the performance of different types of out-of-equilibrium machines converting heat or other forms of energy into useful work.

Specifically, I will consider:

i) an out-of-equilibrium lattice model consisting of 2D discrete rotators, in contact with heath reservoirs at different temperatures,

ii) an out-of-equilibrium Frenkel–Kontorova model moving over a periodic substrate and in a position dependent temperature profile,

iii) a transverse field Ising model undergoing a quantum phase transition, and operating as a battery-charger system.

For each of these systems, I will argue that the optimal operating regime occurs when the system is driven out-of-equilibrium in proximity of a phase transition.

Tuesday 28/09, 09:30 – 09:50

Thermodynamic uncertainty relations for many-body systems with fast jump rates and large occupancies

Ohad Shpielberg [1] and Arnab Pal [2]

CT

[1] *University of Haifa*

[2] *Indian Institute of Technology Kanpur*

A universal large $\mathcal{N}$ theory of nonequilibrium fluctuations emerges in the limit of fast jump rates and large occupancies. We use this theory to derive a set of coarse grained thermodynamic uncertainty relations (TUR) – one of them being an activity bound. Importantly, the activity serves as a tighter bound for the entropy production in 1D systems. These results are particularly useful in the many-body regime, where typically a coarse grained approach is required to handle the large microscopic state space. The work is available on the arXiv `https://arxiv.org/abs/2108.09979`

Tuesday 28/09, 09:50 – 10:10

Non-Markovianity boosting the performance of a quantum Otto engine

Krzysztof Ptaszyński CT

Institute of Molecular Physics, Polish Academy of Sciences, Mariana Smoluchowskiego 17, 60-179 Poznań

It is investigated whether the non-Markovianity, i.e., the memory effects resulting from the coupling of the system to its environment, can be beneficial for the performance of quantum heat engines. Specifically, a version of a single-qubit Otto engine is studied in which the standard thermalization strokes are replaced with so-called extremal thermal operations, which cannot be realized without the memory effects [1]. The performance of such a device is compared with both the Markovian (memoryless) Otto engine and the three-stroke engine studied by Łobejko *et al.* [2], in which the cycle consists of two extremal thermal operations and a single qubit rotation. It is first demonstrated that the non-Markovian Otto engine can generate more work per cycle for a given efficiency than its Markovian counterpart, which, on the other hand, exceeds the performance of the three-stroke engine. Secondly, the ratio of the work fluctuations to the mean work is analyzed. It is shown that both the non-Markovian Otto engine and the three-stroke engine produce less work fluctuations than the Markovian setup (thus providing a more stable operation), whereas their relative performance depends on the target efficiency and work-per-cycle. This leads to the conclusion that the non-Markovian effects can improve the performance of quantum heat engines.

References

[1] E. A. Aguilar, H. Wojewódka-Ściążko, M. Stankiewicz, C. Perry, P. Ćwikliński, A. Grudka, K. Horodecki, and M. Horodecki, arXiv:2009.03110 (2020).

[2] M. Łobejko, P. Mazurek, and M. Horodecki, Quantum **4**, 375 (2020).

Tuesday 28/09, 10:10 – 10:30

Fast is hot: energetics of information erasure and the overhead to Landauer's bound

Salambô Dago [1], Ludovic Bellon [1], Jorge Pereda [1] and Sergio Ciliberto [1]

CT

[1] *Laboratoire de Physique de l'ENS de LYON*

Information processing in the physical world comes with an energetic cost: Landauer's principle states that erasing a 1-bit memory requires at least $k_B T_0 \ln 2$ of energy, with $k_B T_0$ the thermal energy of the surrounding bath. Practical erasures implementations require an overhead to the Landauer's bound, observed to scale as $k_B T_0 B/\tau$, with τ the protocol duration and B close to the system relaxation time. Most experiments use overdamped systems, for which minimizing the overhead means minimizing the dissipation. Underdamped systems, never harnessed before, thus sounds appealing to reduce this energetic cost.

We use as one-bit memory an underdamped micro-mechanical oscillator confined in a double-well potential created by a feedback loop. The potential barrier is precisely tunable in the few $k_B T_0$ range. We measure, within the stochastic thermodynamic framework, the work and the heat of the erasure protocol. We demonstrate experimentally and theoretically that, in this underdamped system, the Landauer's bound is reached within a 1% uncertainty, with protocols as short as 100 ms.

Furthermore, we show that for such underdamped systems, fast erasures induce a heating of the memory: the work influx is not instantaneously compensated by the inefficient heat transfert to the thermostat. This temperature rise results in a kinetic energy contribution superseding the viscous dissipation term. Our model covering all damping regimes paves the way to new optimisation strategies in information processing, based on the thorough understanding of the energy exchanges. We are indeed able to quantify the overhead to the Landauer's bound with its dependence on the system and protocol parameters, and we identify the physical origins of this energy cost.

Tuesday 28/09, 10:30 – 10:50

"Private Truths, Public Lies" within agent-based modeling

Katarzyna Sznajd-Weron CT

Wroclaw University of Science and Technology

The title of this work is inspired by the Timur Kuran's book entitled "Private Truths, Public Lies. The Social Consequences of Preference Falsification". During my presentation I will talk about the idea and real-life examples of Preference Falsification (PF). Furthermore, I will propose a binary agent-based model, which allows to describe PF by introducing two levels of the opinion: the public and the private one. Finally, I will discuss how PF can help in explaining social and political dynamics.

Tuesday 28/09, 10:50 – 10:55

Stochastic thermodynamics of anomalous diffusion generated by scaled and fractional Brownian motions

Seyed Mohsen Jebreiil Khadem [1], Rainer Klages [2] and Sabine H. L. Klapp [1]

[1] *Institute for Theoretical Physics, Technical University of Berlin*

[2] *Queen Mary University of London*

FT

We study stochastic thermodynamics for non-equilibrium systems that can exhibit anomalous diffusion with the main focus on deriving an integral fluctuation relation (IFR) for the total entropy production. The dynamics of those systems are described by (i) Markovian processes with a time-dependent diffusivity such as scaled Brownian motion and (ii) non-Markovian fractional Brownian motion. The former case is an immediate generalization of normal diffusion which is used here mainly, first, to generalize the definitions of the thermodynamic quantities such as heat, work and entropy production along a single trajectory and, second, to revisit the derivation of the IFR for the total entropy production by considering that the fluctuation-dissipation relation may or may not be valid. In the latter case, we investigate how the non-Markovian feature of the dynamics alters the conventional notion of stochastic thermodynamics by leading to a violation of the IFR for the total entropy production. We demonstrate that, such a violation can be circumvented by formally defining a temperature functional that fulfils a general form of fluctuation-dissipation relation. Using a perturbation method, we calculate the first two leading terms of the temperature functional. Our perturbative analysis also unravels that the origin of that violation can be tracked to a generalized form of a heat exchange between the system and the environment. We obtain an analytical expression for the generalized heat function and provide a physically meaningful interpretation by introducing the concepts of retarded force and retarded velocity that include the impact of the memory of the environment.

Tuesday 28/09, 10:55 – 11:00

The q-neighbor Ising model on multiplex networks with partial overlap

Andrzej Krawiecki [1] and Tomasz Gradowski [1]

FT

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

The q-neighbor Ising model is considered on multiplex networks with two layers in the form of identical random graphs, in which only a fraction of nodes belongs to both layers, forming the overlap. In this model the probability of the spin flip for a node belonging only to one layer is given by the Metropolis-like formula with the local field depending on the states of its q randomly chosen neighbors within this layer, and for a node belonging to the overlap is a product of the above-mentioned probabilities for the two layers. Critical properties of the model for varying temperature depend on the size of the neighborhood q and of the overlap r as well as on the mean degree of nodes $\langle k \rangle$ within the layers. For large $\langle k \rangle$ results for the model on multiplex networks with layers in the form of complete graphs are reproduced which can be explained using mean-field approximation [A. Chmiel *et al.*, Phys. Rev. E 96, 062137 (2017)]. In particular, for $q = 2$ for large enough r including complete overlap first-order ferromagnetic transition occurs, for a narrow interval of smaller r the paramagnetic and ferromagnetic phases coexist for temperature decreasing to zero, and for small r the paramagnetic phase is stable for any temperature; and for $q \geq 4$ the ferromagnetic transition is first-order for small r and second-order for larger r including complete overlap. As $\langle k \rangle$ is decreased, for $q = 2$ first-order transition and coexistence of the paramagnetic and ferromagnetic phase occurs at smaller r, and for large and complete overlap second-order ferromagnetic transition appears; and for $q \geq 4$ the interval of small r for which first-order transition occurs becomes narrower. Results of Monte Carlo simulations for the model on multiplex networks with layers in the form of random regular graphs show good quantitative agreement with predictions of the homogeneous pair approximation. Such agreement is remarkable since the latter approximation takes into account only heterogeneity of the nodes due to their location within or outside the overlap, while the density of active links connecting spins with opposite orientation is assumed uniform within each layer.

Symposium will take place according to
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Session 5

Tuesday 28/09, 12:00 – 12:30

Elastohydrodynamics of microscale swimming

Maciej Lisicki IT

Institute of Theoretical Physics, Faculty of Physics, University of Warsaw

Swimming microorganisms and engineered artificial swimmers use multiple strategies to achieve propulsion in the viscosity-dominated microworld. A number of them use long, filamentous appendages called cilia or flagella. The motion of these slender objects is governed by a complex interplay between the driving forces, the elastic properties of the fibres, and the resistance forces of fluid. In my talk, I will describe the basic ideas behind microscale swimming and highlight the role of elastic flagella in swimming. I will show examples of both natural swimmers and artificial systems which can be described using elastohydrodynamics.

A recently studied system involving an emulsion of microscopic droplets of oil in water exhibits swimming induced by an extrusion of elastic fibres by the droplets [1]. The extrusion is controlled by a surface phase transition of the surfactant, and it drives the motion of droplets. Extruded fibres undergo dynamic buckling and produce complex shapes, which we describe by a combination of theoretical modelling and numerical simulations, which serve as the basis for interpretation of experimental data.

[1] D. Cholakova, M. Lisicki, S.K. Smoukov, S. Tcholakova, E. Lin, J. Chen, G. De Canio, E. Lauga, N. Denkov, *Rechargeable self-assembled droplet microswimmers driven by surface phase transitions*, Nature Physics (2021).

Tuesday 28/09, 12:30 – 12:50

Paradigm shift in diffusion-mediated surface phenomena

Denis Grebenkov CT

CNRS

Diffusion-mediated surface phenomena are crucial for human life and industry, with examples ranging from oxygen capture by lung alveolar surface to heterogeneous catalysis, gene regulation, membrane permeation and filtration processes. Their current description via diffusion equations with mixed boundary conditions is limited to simple surface reactions with infinite or constant reactivity. In this talk, we present a probabilistic approach based on the concept of boundary local time [1] to investigate the intricate dynamics of diffusing particles near a reactive surface [2]. Reformulating surface-particle interactions in terms of stopping conditions, we obtain in a unified way major diffusion-reaction characteristics such as the propagator, the survival probability, the first-passage time distribution, and the reaction rate [3-5]. This general formalism allows us to describe new surface reaction mechanisms such as for instance surface reactivity depending on the number of encounters with the diffusing particle that can model the effects of catalyst fooling or membrane degradation. The disentanglement of the geometric structure of the medium from surface reactivity opens far-reaching perspectives for modeling, optimization and control of diffusion-mediated surface phenomena.

References:
[1] D. S. Grebenkov, Phys. Rev. E 100, 062110 (2019)
[2] D. S. Grebenkov, Phys. Rev. E 102, 032125 (2020)
[3] D. S. Grebenkov, Phys. Rev. Lett. 125, 078102 (2020)
[4] D. S. Grebenkov, J. Stat. Mech. 103205 (2020)
[5] D. S. Grebenkov, J. Phys. A.: Math. Theor. 54, 015003 (2021)

Tuesday 28/09, 12:50 – 13:10

Integral decomposition for the solutions of the generalized Cattaneo equation

Katarzyna Górska CT

Institute of Nuclear Physics, Polish Academy of Sciences

We present the integral decomposition for the fundamental solution of the generalized Cattaneo equation with both time derivatives smeared through convoluting them with some memory kernels. For power-law kernels $t^{-\alpha}$, $\alpha \in (0,1]$ this equation becomes the time fractional one governed by the Caputo derivatives in which the highest order is 2.To invert the solutions from the Fourier-Laplace domain to the space-time domain we use analytic methods based on the Efross theorem and find out that solutions looked for are represented by integral decompositions which tangle the fundamental solution of the standard Cattaneo equation with nonnegative and normalizable functions being uniquely dependent on the memory kernels. Furthermore, the use of methodology arising from the theory of complete Bernstein functions allows us to assign such constructed integral decompositions the interpretation of subordination. This fact is preserved in two limit cases built into the generalized Cattaneo equations, i.e., either the diffusion or the wave equations. We point out that applying the Efross theorem enables us to go beyond the standard approach which usually leads to the integral decompositions involving the Gaussian distribution describing the Brownian motion. Our approach clarifies puzzling situation which takes place for the power-law kernels $t^{-\alpha}$ for which the subordination based on the Brownian motion does not work if $\alpha \in (1/2,1]$.

[1] K. Górska, Integral decomposition for the solutions of the generalized Cattaneo equation, Phys. Rev. E 104 (2021) 024113
[2] K. Górska, A. Horzela, E. K. Lenzi, G. Pagnini, T. Sandev, Generalized Cattaneo (telegrapher's) equations in modeling anomalous diffusion phenomena, Phys. Rev. E 102 (2020) 022128

Tuesday 28/09, 13:10 – 13:30

Resonances in Electron Scattering by Molecules

Serg Pozdneev CT

P.N.Lebedev Physical Institute

The methods of the quantum theory few-body scattering based on the Faddeev-Yakubovsky equations [1] in momentum and configuration space are present [1,2]. Scattering states properties of three-body resonantly interacting particles are considered and are shown to be independent of a form of two-body forces, being determined only presence of resonances. The resonances produce an effective long range interaction between three particles [1-2]. This methods are applied to the calculation of the dissociative electron attachment to hydrogen and hydrogen-halide diatomic initial rovibrational exiting molecules H_2, N_2, Li_2, Na_2, HCl, DCl, HBr, DBr, HJ, DJ.

References:
[1] Faddeev L D and Merkuriev S P 1983 Quantum scattering theory for several particles systems, Kluwer, London.
[2] Pozdneev S A 2001 Application on the quantum theory of few-body scattering to the calculation of the different processes in nuclear, atomic and molecular physics, Moscow, Janus-K.

Tuesday 28/09, 13:30 – 13:35

Stochastic jetting and dripping in confined soft granular flows

Michał Bogdan [1], Andrea Montessori , Adriano Tiribocchi [2] , Fabio Bonaccorso [2] , Marco Lauricella [2] , Sauro Succi [2] and Jan Guzowski [1]

FT

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

[2] *Istituto per le Applicazioni del Calcolo del Consiglio Nazionale delle Ricerche*

We report new dynamical modes in confined soft granular flows, such as stochastic jetting and dripping, with no counterpart in continuum viscous fluids. The new modes emerge from an avalanche-like dynamics of a close-packed monodisperse emulsion entering a narrow orifice. We observe formation of remarkably stable single-file granular jets which occasionally break resulting in non-Gaussian distribution of cluster sizes. We find that the sequences of droplet rearrangements that lead to the formation of such chains resemble unfolding of cancer cell clusters in narrow capillaries, overall demonstrating that the microfluidic emulsion systems could serve to model certain aspects of tissue dynamics.

Tuesday 28/09, 13:35 – 13:40

Diffraction and interference with run-and-tumble particles

Kasper Meerts

FT

KU Leuven

Run-and-tumble particles, frequently considered today for modeling bacterial locomotion, naturally appear outside a biological context as well, e.g. for producing waves in the telegraph process. Here, we use a wave function to drive their propulsion and tumbling. Such quantum-active motion realizes a jittery motion of Dirac electrons (as in the famous Zitterbewegung): the Dirac electron is a run-and-tumble particle, where the tumbling is between chiralities. We visualize the trajectories in diffraction and double slit experiments for electrons. In particular, that yields the time-of-arrival statistics of the electrons at the screen. Finally, we observe that away from pure quantum guidance, run-and-tumble particles with suitable spacetime-dependent parameters produce an interference pattern as well.

Symposium will take place according to
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Session 6

Tuesday 28/09, 16:00 – 16:30

Accumulation time of stochastic processes with resetting

Paul Bressloff IT

Department of Mathematics, University of Utah

One of the characteristic features of a stochastic process under resetting is that the probability density converges to a non-equilibrium stationary state (NESS). In addition, the approach to the stationary state exhibits a dynamical phase transition, which can be interpreted as a traveling front separating spatial regions for which the probability density has relaxed to the NESS from those where transients persist. A very different mechanism for generating an NESS occurs within the context of diffusion-based morphogenesis, in which an extrinsic localized current source combined with degradation within the interior of the domain leads to the formation of a protein concentration gradient. A common method for characterizing the relaxation process is to calculate the so-called accumulation time. The latter is the analog of the mean first passage time of a search process, in which the survival probability density is replaced by an accumulation fraction density. In this paper, we extend the definition of the accumulation time to stochastic processes with resetting by showing how the probability density associated with trajectories that reset at least once evolves in an analogous fashion to protein concentration gradients. We consider a range of examples, including diffusion with instantaneous resetting, resetting with refractory periods and finite return times, and non-diffusive processes such as run-and-tumble particles. In each case we calculate the accumulation time as a function of the spatial separation from the reset point.

Tuesday 28/09, 16:30 – 16:50

Geometric Brownian Motion under Stochastic Resetting: A Stationary yet Non-ergodic Process

Viktor Stojkoski [1], Trifce Sandev [1], Arnab Pal [2] and Ljupco Kocarev [1]

CT

[1] *Macedonian Academy of Sciences and Arts*

[2] *Indian Institute of Technology Kanpur*

We study the effects of stochastic resetting on geometric Brownian motion (GBM), a canonical stochastic multiplicative process for non-stationary and non-ergodic dynamics. Resetting is a sudden interruption of a process, which consecutively renews its dynamics. We show that, although resetting renders GBM stationary, the resulting process remains non-ergodic. Quite surprisingly, the effect of resetting is pivotal in manifesting the non-ergodic behavior. In particular, we observe three different long-time regimes: a quenched state, an unstable and a stable annealed state depending on the resetting strength. Notably, in the last regime, the system is self-averaging and thus the sample average will always mimic ergodic behavior establishing a stand alone feature for GBM under resetting. Crucially, the above-mentioned regimes are well separated by a self-averaging time period which can be minimized by an optimal resetting rate. Our results can be useful to interpret data emanating from stock market collapse or reconstitution of investment portfolios.

Tuesday 28/09, 16:50 – 17:10

Random amplitude stochastic resetting

Marcus Dahlenburg [1], Ralf Metzler [2], Aleksei Chechkin [2] and Rina Schumer [3]

CT

[1] *Basque Center for Applied Mathematics: BCAM*

[2] *University of Potsdam*

[3] *Desert Research Institute, Reno*

Stochastic resetting is a stochastic process that is reset randomly in time to its initial position and it is used in many applications as a search strategy.

In my talk I will introduce a model whose resetting events have a random amplitude instead of a back-step to the origin [1]. In particular, we study and discuss two classes of random-amplitude stochastic resetting: independent and dependent resetting. Independent resetting is characterized by amplitudes that are unconditioned to the resetting events, which occur in the opposite direction with respect to the average free-propagation. Dependent resetting amplitudes have in turn limits on the system states such that the particle may be only partially reset towards the trajectory's origin. Independent resetting is a non-stationary stochastic process which may overshoot the initial position, whose mean and variance show a linear growth in time, while dependent resetting is a generalization of stochastic resetting and is a stationary stochastic process. Geophysical layering (Stratigraphy) and population dynamic are direct applications for both classes of random-amplitude stochastic resetting.

1. M. Dahlenburg, A. V. Chechkin, R. Schumer, and R. Metzler, Stochastic resetting by a random amplitude, Phys. Rev. E, 103, 052123 (2021)

Tuesday 28/09, 17:10 – 17:30

The role of the Laplace distribution in stochastic resetting

Aleksander Stanislavsky CT

Faculty of Pure and Applied Mathematics, Hugo Steinhaus Center, Wroclaw University of Science and Technology

Diffusion with stochastic resetting is very popular in the study of many phenomena in physics, biophysics, chemistry. A wide diversity of random processes and restart mechanisms are widespread in nature, science and technology. As a stochastic process under resetting, we consider a subordinated Brownian process, and the restart time is exponentially distributed with constant rate. In this case the stationary state has the Laplace distribution in which the scaling parameter is dependent on the Laplace exponent of the random process directing Brownian motion as a parent process. The directing process may be taken from a wide set of infinitely divisible random processes. Changing the subordinator, we can modify the parameter, but the stationary state still obeys the Laplace distribution. If the linear potential acts on the subordinated Brownian motion under resetting, this leads to an asymmetric form of the Laplace distribution. If Brownian motion becomes Lévy flights, due to resetting the stationary state has the Linnik distribution, generalizing the Laplace case in the sense of geometrically infinitely divisible distributions. This analysis includes the ordinary diffusion with resetting as a particular example.

Tuesday 28/09, 17:30 – 17:50

Gut's complexity

Dante R. Chialvo CT

Center for Complex Systems and Brain Sciences, Instituto de Ciencias Físicas, Universidad Nacional de San Martin , (Argentina)

Our guts host one of the largest interaction network, only comparable in size and complexity with the nervous and the inmune systems. The intricacy of its organization it just started to be unveiled as novel DNA technology provides data. We will describe our most recent efforts in that direction.

Tuesday 28/09, 17:50 – 17:55

First passage under restart for discrete space and time

Ofek Lauber [1] and Arnab Pal [2]

FT

[1] *Tel Aviv University*

[2] *IIT, Kanpur, India*

First passage under restart has recently emerged as a conceptual framework to study various stochastic processes under a restart mechanism. Restart has been shown to expedite the completion of many first passage processes which otherwise would take a longer time to finish. However, most of the studies so far focused on continuous time and space, while discrete processes received less attention. In this talk, I will bridge this gap by presenting a renewal approach for studying discrete space and time first passage processes under discrete time resetting. Using this general set-up, I compute the moments and the probability mass function of the restarted first passage time and derive a sufficient criterion for geometric restart to be beneficial. I will demonstrate the usefulness of this method by applying it to one-dimensional lattice random walks in confined geometry.

References

[1] Bonomo, O.L. and Pal, A., 2021. First passage under restart for discrete space and time: Application to one-dimensional confined lattice random walks. Physical Review E, 103(5), p.052129.
[2] Bonomo, O.L. and Pal, A., 2021. The P\'{o} lya and Sisyphus lattice random walks with resetting–a first passage under restart approach. arXiv preprint arXiv:2106.14036.

Tuesday 28/09, 17:55 – 18:00

Bayesian inference of Lévy walks via hidden Markov models: parameter estimation and model classification

Seongyu Park [1], Samudrajit Thapa [2], Michael Lomholt [3],
Jae-Hyung Jeon [1] and Yeongjin Kim [1]

FT

[1] *Pohang University of Science and Technology*

[2] *Tel Aviv University*

[3] *University of Southern Denmark*

Lévy walk is a non-Markovian anomalous diffusion model that has been widely used to describe random walks in diverse fields such as biology, quantum physics, and ecology. One of the controversial issues in these fields is that whether the given diffusion dynamics can be successfully explained by a Lévy walk or not, which becomes a nontrivial issue if diffusion data is short and noisy. In this work, we propose a Bayesian inference method for model classification and parameter estimation of time trace data of noisy Lévy walks. We propose how to calculate the likelihood function of a Lévy walk, which is a non-Markovian process, via hidden Markov models. With this likelihood function, we carry out the Bayesian model comparison and parameter estimation on the simulated trajectories at various conditions. We demonstrate that the likelihood function is successfully calculated via hidden Markov model, and the Bayesian inference works well for the trajectories with moderate signal-to-noise levels.

Symposium will take place according to
Central European Summer Time (CEST/UTC+2:00/GMT+2:00)

Session 7

Wednesday 29/09, 09:00 – 09:30

Non-Gaussian statistics in soft & bio-matter

Ralf Metzler IT

University of Potsdam

Brownian yet non-Gaussian diffusion, characterised by a linear scaling in time of the mean squared displacement but a non-Gaussian displacement distribution is a phenomenon that has been observed in a variety of systems. In my talk, after a brief historical introduction to Brownian motion and the theory of diffusion, I will review experimental evidence and show how non-Gaussian statistics emerge from random-parameter models, extreme value arguments, and other models. In particular, I will also talk about quenched versus annealed disorder and demonstrate how shape-shifting in tracers leads to time-fluctuating diffusivities. I will finally address anomalous diffusion systems driven by long-ranged correlated Gaussian noise that, in heterogeneous environments, exhibit non-Gaussian displacement distributions.

Wednesday 29/09, 09:30 – 09:50

Unified Approach to Gated Reactions on Networks

Yuval Scher [1] and Shlomi Reuveni [1]

CT

[1] *Tel Aviv University*

For two molecules to react they first have to meet. Yet, reaction times are rarely on par with the first passage times that govern such molecular encounters. A prime reason for this discrepancy is stochastic transitions between reactive and nonreactive molecular states, which results in effective gating of product formation and altered reaction kinetics. To better understand this phenomenon we develop a unifying approach to gated reactions on networks. We first show that the mean and distribution of the gated reaction time can always be expressed in terms of ungated first-passage and return times. This relation between gated and ungated kinetics is then explored to reveal universal features of gated reactions. The latter are exemplified using a diverse set of case studies which are also used to expose the exotic kinetics that arises due to molecular gating.

Wednesday 29/09, 09:50 – 10:10

Epidemic-Driven Collapse in a System with Limited Economic Resource

Oleksandr Kliushnichenko [1], Ivan Gandzha [1] and Sergey Lukyanets [1]

CT

[1] *Institute of Physics, NAS of Ukraine*

We consider the possibility of socioeconomic collapse of the population caused by epidemics spreading. Using a simple model of negative feedback we study the dynamics of epidemic spreading in a group of agents with its mutual influence on some formal resource (economical, financial, etc). A coupling mechanism between spreading- and resource-subsystem is supposed to be governed by over-barrier transitions (Arrhenius-like law) that is possible when economic resource associated with average income per agent formally represents the market temperature and obeys the Boltzmann-Gibbs statistics [1]. We show that depending on the rate of epidemics spreading and on the availability of formal resource, the system can come back to normal life, can overcome the stress, or move to another stable but more "poor" state [2,3]. Otherwise, in the case of limited recourse and non-zero activation energy, the epidemic intensified by the increasing resource deficit can ultimately drive the system to collapse. While collapsing, the system can pass through a number of quasi-stable states, its dynamics being resembling the so-called devil's staircase. We also briefly discuss several mitigation strategies involving financial and social regulations and illustrate the ambiguous effect of quarantine measures.

[1] A. Dragulescu, V.M. Yakovenko, Eur. Phys. J. B **17**, 723 (2000)
[2] I.S. Gandzha, O.V. Kliushnichenko, S.P. Lukyanets, Eur. Phys. J. B **94**, 90 (2021)
[3] I.S. Gandzha, O.V. Kliushnichenko, S.P. Lukyanets, Chaos, Solitons & Fractals **148**, 111046 (2021)

Wednesday 29/09, 10:10 – 10:30

Extinctions of coupled populations, and rare event dynamics under non-Gaussian noise

Tal Agranov [1] and Guy Bunin [2]

CT

[1] *University of Cambridge*

[2] *Technion - Israel Institute of Technology*

The survival of natural populations may be greatly affected by environmental conditions that vary in space and time. We look at a population residing in two locations (patches) coupled by migration, in which the local conditions fluctuate in time. We report on two findings. First, we find that, unlike rare events in many other systems, here the histories leading to a rare extinction event are not dominated by a single path. We develop the appropriate framework, which turns out to be a hybrid of the standard saddle-point method and the Donsker-Varadhan formalism which treats rare events of atypical averages over a long time. It provides a detailed description of the statistics of histories leading to the rare event and the mean time to extinction. The framework applies to rare events in a broad class of systems driven by non-Gaussian noise. Second, applying this framework to the population-dynamics model, we find a phase transition in its extinction behavior. Strikingly, a patch which is a sink (where individuals die more than are born) can nonetheless reduce the probability of extinction, even if it lowers the average population's size and growth rate.

Wednesday 29/09, 10:30 – 10:50

The mechanics of domain formation in the gene expression profiles

Maciej Majka CT

Institute of Theoretical Physics, Jagiellonian University, Kraków, Poland

In embryo development, cells specialize into their future role by changing their gene expression levels in response to the concentrations of competing chemical signals, called morphogens. This paradigm is known as Wolpert's French flag model. In the mathematical modelling of these phenomena, a profound role is played by the reaction-diffusion equations involving some form of activation term (i.e. the Hill function). Yet, even the numerical analysis of these models is usually challenging due to their non-linear nature and large number of parameters involved. In this presentation, I will discuss the analytical solution to the generic model of domain formation, based on diffusion equations with a theta Heaviside activation term. The solution reveals a phase transition in the domain formation and allows for an exact insight into the dynamics of activation fronts and the conditions for stabilization of activated domains. This will be discussed using the example of two mutually repressive genes.

Wednesday 29/09, 10:50 – 10:55

Achieving robustness and precision in the developing spinal cord with system-level feedback

Richard Ho [1], Maciej Majka [1], Marcin Zagórski [1] and Adela Staszowska [1]

FT

[1] *Institute of Theoretical Physics, Jagiellonian University, Kraków, Poland*

Spinal cord development is a complex process due to the interplay of signaling molecules over varying length and time scales. Despite the intrinsic stochasticity of signaling events, the resulting pattern of gene expression domains is remarkably precise and reproducible between individuals. How this patterning precision is achieved is still poorly understood. By investigating formation of source region (floor plate, FP) that secrets signaling molecules (morphogen, Shh), the spread of these molecules across growing tissue and the interpretation of resulting cellular signaling by gene network we want to identify the system-level feedback driving precise pattern formation. We use a thermodynamic model coupled with reaction-diffusion equation to describe inter-regulation of FP, target genes and spreading of Shh molecules. We define a success criteria for simulations, and examine the robustness, size of FP, and time evolution of these successful simulations to make predictions for the biological system. We find that the system development can be divided into two phases, and we then attempt to delineate which model parameters most affect which of these two phases. We also find that longer FP is associated with lower robustness to stochastic noise but greater robustness to changes in initial conditions suggesting the existence of an interesting trade-off.

Wednesday 29/09, 10:55 – 11:00

Collagen as Hopf's fibration

Ryszard Wojnar FT

Institute of Fundamental Technological Research PAS

The shape of many biomolecules is similar to the Coxeter-Boerdijk (CB) helix, made of tetrahedra placed next to each other in such a way that the tetrahedrons are adjacent to each other with their faces. The helix CB is the solution to the maximum packing task. In the collagen helix, every third amino acid is glycine (Gly), and the entire chain contains primarily proline (Pro). Half of the Pro groups are hydroxyproline (Hyp). Each collagen chain contains the repeating components of Gly-X-Y, with X or Y being almost always Pro or Hyp. That is why a single chain of collagen itself is called proline. Proline is also found in biomolecules other than collagen. In collagen, the 3 proline (left-handed) helices fold into one right-handed helix. The chain of tetrahedra of the CB helix can be detected in a polytope (3, 3, 5). It is the regular structure similar to the S3 hypersphere built of 600 tetrahedra. The 600-cell can be decomposed over 25 overlapping 24-cells. The vertices of this structure, numbering 120, are arranged 10 on the 12 non-intersecting great circles of the hypersphere. These great circles are Hopf S3 fibration fibers, each fiber having 10 vertices.
While the structure of biological molecules seems complicated, their topology turns out to be simple thanks to spatial considerations, as a result of which it turns out that mathematical helices have geometrical properties of biological helices.

Symposium will take place according to
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Session 8

Wednesday 29/09, 12:00 – 12:30

Enhancing transport by shaping barriers (beating activation energies)

Emmanuel Trizac IT

Université Paris-Saclay

Brownian escape is key to a wealth of physico-chemical processes, including polymer folding and information storage. The frequency of thermally activated energy barrier crossings is assumed to generally decrease exponentially with increasing barrier height. Here, we show theoretically and experiment tally that higher, fine-tuned barrier profiles result in significantly enhanced escape rates, in breach of the intuition relying on the above scaling law, and address the corresponding conditions for maximum speed-up.

Wednesday 29/09, 12:30 – 13:00

Colossal Brownian, yet non-Gaussian diffusion in a periodic potential

Jakub Spiechowicz IT

University of Silesia

I will report on a novel class of Brownian, yet non-Gaussian diffusion, in which the mean square displacement of the particle grows linearly with time, the probability density for the particle spreading is Gaussian like, but the probability distribution for its position increments possesses an exponentially decaying tail. In contrast to recent works in this area, this behavior is not a consequence of either a space- or time-dependent diffusivity, but is induced by external non-thermal noise acting on the particle dwelling in a periodic potential. The exponential tail in the increment statistics leads to colossal enhancement of diffusion, drastically surpassing the previously researched situation known as “giant” diffusion.

Wednesday 29/09, 13:00 – 13:20

Interacting Persistent Random Walkers

Martin Evans CT

University of Edinburgh

In this talk I will consider persistent random walkers, also known as run and tumble particles, which are emerging as a fundamental microscopic model of active matter. I will review the properties of a single persistent walker then consider the case of two persistent random walkers that interact through an exclusion interaction. An exact expression for the stationary state of two such walkers on a periodic lattice reveals how the particles jam and generate an effective attractive potential. The full spectrum of the two-particle problem can also be computed and exhibits exceptional points, which correspond to dynamical transitions in the relaxation time.

Jamming and attraction of interacting run-and-tumble random walkers, AB Slowman, MR Evans, RA Blythe, Physical review letters 116 (21), 218101 (2016)

Exact spectral solution of two interacting run-and-tumble particles on a ring lattice, E Mallmin, RA Blythe, MR Evans, Journal of Statistical Mechanics: Theory and Experiment 2019 (1), 013204

Wednesday 29/09, 13:20 – 13:40

Should I stay or should I go? Zero-size jumps in random walks for Lévy flights

Gianni Pagnini [1] and Silvia Vitali [1]

CT

[1] *BCAM - Basque Center for Applied Mathematics*

Motivated by the fact that, in the literature dedicated to random walks for anomalous diffusion, it is disregarded if the walker does not move in the majority of the iterations because the most frequent jump-size is zero (i.e., the jump-size distribution is unimodal with mode located in zero) or, in opposition, if the walker always moves because the jumps with zero-size never occur (i.e., the jump-size distribution is bi-modal and equal to zero in zero), we provide an example in which indeed the shape of the jump-distribution plays a role.
In particular, we show that the convergence of Markovian continuous-time random walk (CTRW) models for Lévy flights to a density function that solves the fractional diffusion equation is not guaranteed when the jumps follow a bi-modal power-law distribution equal to zero in zero, but, as a matter of fact, the resulting diffusive process converges to a density function that solves a double-order fractional diffusion equation.
Within this framework, self-similarity is lost. The consequence of this loss of self-similarity is the emergence of a time-scale for realizing the large-time limit. Such time-scale results to span from zero to infinity accordingly to the power-law displayed by the tails of the walker's density function. Hence, the large-time limit could not be reached in real systems.
The significance of this result is two-fold: i) with regard to the probabilistic derivation of the fractional diffusion equation and also ii) with regard to recurrence and the related concept of site fidelity in the framework of Lévy-like motion for wild animals.

Talk based on:
G. Pagnini and S. Vitali. Should I stay or should I go? Zero-size jumps in random walks for Lévy flights, Fract. Calc. Appl. Anal., 24(1), 137–167, 2021.

Wednesday 29/09, 13:40 – 14:00

Inertial Lévy flights in bounded domains

Karol Capała [1] and Bartłomiej Dybiec [1]

CT

[1] *Institute of Theoretical Physics, Jagiellonian University, Kraków, Poland*

The escape from a given domain is one of the fundamental problems in statistical physics and the theory of stochastic processes. In this talk we will explore properties of the escape of an inertial particle driven by Lévy noise from a bounded domain, restricted by two absorbing boundaries. The properties of the mean first passage time for the integrated Ornstein–Uhlenbeck process driven by Lévy noise will be compared to its Brownian counterpart i.e. randomly accelerated process. Mean first passage time considerations will be complemented by analysis of the escape velocity and energy along with their sensitivity to initial conditions.

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Session 9

Wednesday 29/09, 16:00 – 16:30

Dynamic crossover in homogeneous active matter

Tomás S. Grigera IT

IFLySiB – University of La Plata

The dynamic critical behaviour of active matter systems is of theoretical interest in itself but also because of its relevance to swarming in biological groups, where the dynamic critical exponent can be an element to discriminate between alternative models. Here we study the crossover between the equilibrium and off-equilibrium dynamic universality classes in the Vicsek model near its ordering transition. Building on the incompressible hydrodynamic theory of Chen et al. [New J. Phys. **17,** 042002 (2015)], we show that increasing activity leads to a renormalization group (RG) crossover between the equilibrium ferromagnetic fixed point (with dynamical critical exponent $z = 2$) and an off-equilibrium active fixed point (with $z \approx 1.7$ in $d = 3$). We show in numerical simulations that the classic Vicsek model in the near-ordering regime displays a change in the effective dynamical exponent as speed is increased, in in remarkable agreement with the RG prediction. Finally we show that the equilibrium to off-equilibrium crossover is ruled by a characteristic length scale, beyond which active dynamics takes over.

Wednesday 29/09, 16:30 – 16:50

Brownian yet non-Gaussian diffusion in models of disordered systems

Igor Sokolov CT

Humbold University, Berlin

Experimental possibility of single particle tracking on molecular scales lead to a splash of interest to the precise forms of the probability density functions (PDFs) of displacements of classical particles diffusing in complex environments. This lead to the discovery of an intriguing phenomenon of Brownian yet non-Gaussian diffusion in which these PDFs are strongly non-Gaussian (at least at short times, when they typically have a tent-like shape) with slow convergence to Gaussian at long times, while the mean squared displacement grows linearly in time in the whole time domain, like in normal diffusion. The phenomenon is probably not mono-causal, and several models for this were proposed. These models can be roughly divided into two classes: the ones with time-dependent (fluctuating) diffusivity, and the ones, in which diffusion in static, correlated random environments is considered. We show that the behavior of the PDF in these two classes of models during the convergence to a Gaussian is very different.

In models of fluctuating diffusivities, like in usual diffusion, the concentration profile, starting from an initial distribution showing sharp features, rapidly gets smooth and then converges to a Gaussian. The art of convergence to a Gaussian in diffusion in disordered media with infinite contrast may be strikingly different: sharp features of initial distribution do not smooth out at long times and persist indefinitely. This peculiarity of the strong disorder may be of importance for diagnostics of disorder in complex, e.g. biological, systems.

Wednesday 29/09, 16:50 – 17:10

Simulation and tracking of fractional particles motion. From microscopy video to statistical analysis. A Brownian bridge approach

Monika Muszkieta CT

Hugo Steinhaus Center, Wroclaw University of Science and Technology

In this talk, we will go through the whole single-particle tracking procedure, from the extraction of trajectories from a microscopy video to the statistical analysis of particles dynamics. We will consider typical problems arising on the experimental as well as image processing level which lead to inaccurate, fragmented trajectories of short length, and propose several strategies for dealing with incomplete data. We will show that, depending on the chosen method, the obtained results might vary significantly, obviously influencing the final conclusions. This is a joint work with J. Janczura and A. Weron.

Wednesday 29/09, 17:10 – 17:30

Detecting Transient Trapping from a Single Trajectory: A Structural Approach

Yann Lanoiselée [1], Jak Grimes [1], Zsombor Koszegi [1] and Davide Calebiro [1]

[1] *University of Birmingham*

We introduce a new method to detect transient trapping events within a single particle trajectory, thus allowing the explicit accounting of changes in the particle's dynamics over time. Our method is based on new measures of a smoothed recurrence matrix. The newly introduced set of measures takes into account both the spatial and temporal structure of the trajectory. Therefore, it is adapted to study short-lived trapping domains that are not visited by multiple trajectories. Contrary to most existing methods, it does not rely on using a window, sliding along the trajectory, but rather investigates the trajectory as a whole. This method provides useful information to study intracellular and plasma membrane compartmentalisation. Additionally, this method is applied to single particle trajectory data of β2 -adrenergic receptors, revealing that receptor stimulation results in increased trapping of receptors in defined domains, without changing the heterogeneous diffusion of free receptors.

Wednesday 29/09, 17:30 – 17:50

How fast is the ECG signal and why do we need a kinetic theory of conductance

Teodor Buchner CT

Faculty of Physics, Warsaw University of Technology

Human body conducts electricity. It is obvious, but many important details are not. It is argued why the most popular theory of conductance in living tissue is not precise and requires a lot more of physics. The foundations of molecular theory of biopotentials are sketched out and the role of various molecular mechanisms of conductance and polarization is explained. It is shown, that there are many riddles in modern electrodiagnostics which cannot be satisfactorily described with use of present theories. It begins from such basic questions as e.g. the morphology of the T wave, the impact of perfusion on the ECG amplitude, role of ionic strength in signal transmission or the reasons for QRS changes observed after dialysis. There is a growing number of phenomena, which forms an evidence, that a new theory of tissue conductance is required. Solution to many of these riddles may be found in the shape of electric impedance spectra and this is closely related to dielectric spectrum of materials, which for complex materials poses a complex problem. Finally the need for a kinetic theory of polarization in electrolytes is expressed; maybe Smoluchowski-Poisson-Boltzmann can solve the problems? The research was funded by POB Biotechnology and Biomedical Engineering of Warsaw University of Technology within the Excellence Initiative: Research University (IDUB) program 1820/16/Z01/POB4/2021.

Wednesday 29/09, 17:50 – 17:55

Leveraging large deviation statistics to decipher the stochastic properties of measured trajectories

Samudrajit Thapa [1], Agnieszka Wyłomańska [2] , Grzegorz Sikora [2] , Caroline Wagner [3] , Diego Krapf [4] , Holger Kantz [5] , Aleksei Chechkin [6] and Ralf Metzler [6]

FT

[1] *Tel Aviv University*

[2] *Faculty of Pure and Applied Mathematics, Hugo Steinhaus Center, Wrocław University of Science and Technology, Wrocław, Poland*

[3] *Department of Bioengineering, McGill University*

[4] *Department of Electrical and Computer Engineering, Colorado State University*

[5] *Max Planck Institute for the Physics of Complex Systems, Dresden*

[6] *University of Potsdam*

Single-particle tracking routinely measures the motion of different particles in biological and soft-matter systems and often unveils characteristic deviations of the observed stochastic dynamics from standard Brownian motion. To identify the correct underlying physical mechanism often tools such as machine-learning and Bayesian inference are employed. These methods are technically involved and computationally expensive, with the computational cost increasing with the number of models considered. We show that the large-deviation theory applied to the time-averaged mean-squared displacements provides a simple-yet-efficient tool for the construction of decision trees to reject certain models. This facilitates the reduction of the list of feasible models and thereby complements Bayesian and machine-learning methods. We show how we can use this large-deviation theory based approach to uncover additional information from measured trajectories in complex liquids as well as climate data.

Wednesday 29/09, 17:55 – 18:00

The crucial role of inter-trade times in volatility clustering: a continuous-time random walk description

Jarosław Klamut [1] and Tomasz Gubiec [1]

FT

[1] *University of Warsaw*

Continuous-time random walk (CTRW) has found many applications in modelling complex systems dynamics, especially physical or socio-economic phenomena [1]. It is also successfully used to describe the behaviour of prices in the stock markets [2]. Spatial jumps represent price increments and inter-trade times are considered as waiting times. One of the most well-known stylized fact about financial time series is activity clustering regardless of intraday seasonality (lunch effect). Our latest results suggest that these dependencies between waiting times are the key element to explain slowly decaying time autocorrelation of the absolute values of price changes [3].

We introduced a CTRW model in which waiting times come from subordinated CTRW. In this subordinated process, the value (waiting time) is randomly selected and lasts for a random period of time. This results in repeating waiting times in our model. In this way, we can introduce power-law step autocorrelation of waiting times. If the mean increment is nonzero, then time autocorrelation of changes decays like a power-law. In the case of strong memory between waiting times, the process has superdiffusion. The exponents of both step and time autocorrelation are the same. Analytical results were compared with empirical data from Polish stock market.

[1] Kutner, R. & Masoliver, J., *The continuous time random walk, still trendy: fifty-year history, state of art and outlook*, Eur. Phys. J. B (2017) 90:50.
[2] Klamut, J. & Gubiec, T., *Directed continuous-time random walk with memory*, Eur. Phys. J. B (2019) 92:69.
[3] Klamut, J. & Gubiec, T., *Continuous Time Random Walk with correlated waiting times. The crucial role of inter-trade times in volatility clustering*, arXiv:1909.04986v2 (2019).

List of Abstracts – Posters

Poster N° (1)

Active Brownian Motion with Directional Reversals

Ion Santra [1], Urna Basu [1] and Sanjib Sabhapandit [1]

[1] *Raman Research Institute*

Active Brownian motion with intermittent direction reversals are common in a class of bacteria including M. xanthus and P. putida. We show that, for such a motion in two dimensions, the presence of the two time scales set by the rotational diffusion constant D_R and the reversal rate γ gives rise to four distinct dynamical regimes: (I) $t \ll \min(\gamma^{-1}, D_R^{-1})$, (II) $\gamma^{-1} \ll t \ll D_R^{-1}$, (III) $D_R^{-1} \ll t \ll \gamma^{-1}$, and (IV) $t \gg \max(\gamma^{-1}, D_R^{-1})$, showing distinct behaviors. We characterize these behaviors by analytically computing the position distribution and persistence exponents. The position distribution shows a crossover from a strongly non-diffusive and anisotropic behavior at short-times to a diffusive isotropic behavior via an intermediate regime (II) or (III). In regime (II), we show that, the position distribution along the direction orthogonal to the initial orientation is a function of the scaled variable $z \propto x_\perp/t$ with a non-trivial scaling function, $f(z) = (2\pi^3)^{-1/2}\Gamma(1/4 + iz)\Gamma(1/4 - iz)$. Furthermore, by computing the exact first-passage time distribution, we show that a novel persistence exponent $\alpha = 1$ emerges due to the direction reversal in this regime.

Poster N° (2)

Anomalous dynamics governed by a generalized Langevin equation for the active Brownian particle in a viscoelastic polymer environment

Sungmin Joo [1], Xavier Durang [1], HyeongTark Han [1], O-chul Lee [1] and Jae-Hyung Jeon [1]

[1] *Pohang University of Science and Technology*

We study the collective dynamics for a viscoelastic active system where the fluctuation-dissipation theorem (FDT) is violated. We set up a minimal model, where an active Brownian particle (ABP) is cross-linked to a star polymer of functionality f in a viscous fluid. The ABP has self-propelled motion from its own energy consumption and attains a strong non-Markovian anomalous motion due to the viscoelastic feedback from the polymer. We have performed extensive Langevin dynamics simulations on this system at various conditions for two cases in which a star polymer is made up with Rouse chains or worm-like chains (WLC). Our study shows that in the Rouse polymer system the ABP cross-linker with the scaling $\langle \Delta R^2(t) \rangle \sim t^\alpha$ has rich dynamic patterns from the Rouse dynamics ($\sim t^{1/2}$) to logarithmic one ($\sim \ln t$) depending on the strength of self-propulsion[1]. In the WLC environment, the ABP cross-linker shows distinct dynamic behavior. In particular, the seemingly Rouse dynamics can occur due to the active non-equilibrium fluctuation. We explain the observed collective dynamics of the ABP cross-linker in the framework of generalized Langevin equations with two distinct–thermal and athermal–noises.

[1] S. Joo, X. Durang, O.-c. Lee, and J.-H. Jeon, Soft Matter **16**, 9188–9201 (2020)

Poster N° (3)

Collective Dynamical Screening of Disordered Ensembles: Correlation Function, Local Force Fluctuations and Structure Factor

Oleksandr Kliushnichenko [1] and Sergey Lukyanets [1]

[1] *Institute of Physics, NAS of Ukraine*

We study the effects of nonequilibrium correlations and interactions between constituent particles of a bunch, arising under the scattering of particle stream on a cluster or finite cloud of impurities. These induced correlations and dynamical friction forces on impurities are manifested most pronouncedly in the case of collective dynamical screening effect and are enhanced in the case of a nonlinear medium when strong local fluctuations of scattered field begin to act as additional scattering elements due to the collective blockade effect near impurities. In addition, collective scattering effects depend on the degree of impurity cloud disorder. The description of the impurity cluster in terms of effective parameters breaks down due to the presence of strong fluctuations in the spatial distribution of scatterers, besides, quantities characterizing the cluster may lose self-averaging. The presence of strong fluctuations of the scattered field is shown to give rise to strong local fluctuations of nonequilibrium forces acting on certain particles within the impurity cluster that can be a precursor of dynamical instability of the cluster, which is manifested in the peculiar behavior of the tails of probability distribution function for the drag force. The form of appropriate correlation function relating the statistical properties of impurity cloud structure with local forces is discussed. This is to estimate dynamics of impurity cloud in time: stability of moving cluster, the role of local pairing (depletion forces), and possible nonlinear compression of the cluster as a whole.

[1] O.V. Kliushnychenko, S.P. Lukyanets, Phys. Rev. E **95**, 012150 (2017).
[2] O.V. Kliushnychenko, S.P. Lukyanets, Phys. Rev. E **98**, 020101(R) (2018); arXiv: 2012.09266 (2020).

Poster N° 4

Design of structure of sodium alginate membranes filled with iron oxide nanoparticles based on experimental results and simulation of diffusion process

Anna Strzelewicz [1], Monika Krasowska [1], Gabriela Dudek [1] and Michał Cieśla [2]

[1] *Silesian University of Technology*

[2] *Insitute of Theoretical Physics, Jagiellonian University, Kraków, Poland*

For each material, it is possible to individually select the optimal parameters that most accurately describe its unique nature and that influence the features that interest the user. We investigate the morphology of cross-sections of the sodium alginate membranes filled with various amount of magnetite and crosslinked using different agents. 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. Therefore, we try to explore the ways of showing this relationship by simulating the motion of a particle in the membrane environment. In our case, it is a simulation of random walk on the structures of hybrid alginate membranes. Also, for a better understanding of the problem, we model structures of two–dimensional heterogenic membranes which resemble real hybrid alginate structures and then simulate random walk on them. The generated structures of 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 that are comparable to the real hybrid alginate membranes filled with magnetite. Simulations of the particle motion support understanding of the mass transport through polymer materials and give a real chance to find the relation between diffusion and structure properties.

[1] G. Dudek, M. Krasowska, R. Turczyn, M. Gnus, A. Strzelewicz, Sep. Pur. Tech. 182 101 (2017)
[2] M. Krasowska, A. Strzelewicz, G. Dudek, M. Cieśla, Phys. Rev. E 95, 012155 (2017)
[3] A. Strzelewicz, M. Krasowska, G. Dudek, M. Cieśla, Chem. Phys. 531, 110662 (2020)

Poster N° (5)

Application of the few-body quantum theory of scattering for guided control of chemical reaction and creation of the new molecular structures

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Guided control of molecular processes and creation of the new molecular structure is a subject of active research in molecular and chemical physics. One of the most natural and general approaches in this area is a quantum few-body theory based on the Faddeev-Yakubovsky equations [1,2]. It is based on the idea, that the possible mechanisms of occurrence of chemical reactions based on a specific multiparticle interaction under condition of low coupling energy between clasters of the system.

Investigation of the methods and tools for creation of the new molecular structures with new properties and control of chemical reaction on the base quantum theory of few-body system are presented. A general method for study three-body recombination reactions base on Faddeev-Yakubovsky equations is developed. Calculations of the three-body recombination rate of the reactions [2-5] H + H + H $\rightarrow$ H_2+H, He+He+He $\rightarrow$ He_2+He, Cs + +Br - R $\rightarrow$ CsBr + R for low energies are compere with classical results and other approximations.

References:
[1] L.D. Faddeev, S.P Merkuriev Quantum scattering theory for several particles systems, Kluwer, London, 1993.
[2] Pozdneev S.Application of quantum theory of scattiring to the calculations of different processes in nuclear, atomic and molecular physics, Moscow, Janus-K, 2001.

Poster N° 6

Electron scattering by atoms and molecules, multiple scattering approximation, Faddeev-Yakubovsky equations

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The main difficulties in the research of few-body problems are bounded with the really many-channels and multidimensional nature of the these problem, impossible applied many well-known theories such as adiabatic, impulse, coupled hannels, etc. For this reason we proposed new method for the investigation of the different few-body processes used the mathematically rigorous formalism based on the treatment of collision processes as many body processes, using Faddeev-Yakubovsky equations [1,2] (FYE) in integral and differential forms. In particular techniques based on FYE have been used successfully in studies of the dynamics of few-particle systems (bound-state properties and elastic, reactive and breakup scattering) [2]. The following results are presented and discussed. The investigation of the influence of the long range part of pair-wise potentials in FYE on the scattering in few-body systems. The study on the correlation between low-energy characteristic in few-body scattering. The studding the unusual dynamical threshold phenomena in chemical reactions such as Efimov states based on FYE. This research may be obtain the information of the reaction mechanism, PES etc. and may have a strong influence on the scattering observable.

[1] Faddeev L D and Merkuriev S P 1983 Quantum scattering theory for several particles systems, Kluwer, London.

[2] Pozdneev S A 2001 Application on the quantum theory of few-body scattering to the calculation of the different processes in nuclear, atomic and molecular physics, Moscow, Janus-K.

Poster N° (7)

Hopf bifurcation in addition-shattering kinetic equations

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We explore dynamical properties of addition-shattering kinetic equations. For a long time researchers believed that only possible asymptotic regime in closed systems was a steady state. However, stable oscillatory solutions were recently discovered in a series of numerical experiments for a closed system of kinetic equations describing simultaneous aggregation $[i] \oplus [j] \ \to K_{ij}\, [i+j]$ and shattering $[i] \oplus [j] \ \to \lambda \cdot K_{ij}\ \underbrace{[1] + \cdots + [1]}_{i+j}$ processes, where K_{ij} are kinetic rates and weight $0 < \lambda \ll 1$ corresponds to the intensity of shattering.

We attempt to theoretically justify the observed effect and consider a simplified model of the addition-shattering processes. The addition can be represented as $[1] \oplus [s] \ \to A_s\, [1+s]$ and the spontaneous shattering as $[s] \ \to B_s\ \underbrace{[1] + \cdots + [1]}_{s}$. For this system with $A_s = s$ and $B_s = Bs^{\beta}$ we study the stability of the steady-state particle size distribution by studying the eigenvalues of the Jacobi matrix of the nonlinear addition-shattering operator. For a certain region of the parameter space we show the existence of stable persistent oscillatory solutions. They arise when the steady-state particle size distributions lose stability via Hopf bifurcation.

Until now, researchers demonstrated only stationary solutions for aggregation models with linear fragmentation terms but in our work we show that stable oscillations are possible for such class of systems. This work is supported by Russian Science Foundation project 19-11-00338.

[1] Budzinskiy S., Matveev S., Krapivsky P. (2021). Hopf bifurcation in addition-shattering kinetics. PRE, L040101.

Poster N° 8

Influence of a magnetic field on the drainage mechanism of the thin liquid film (TLF) and real foams stabilized by magneto-reactive surfactants

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Foam is a dispersed system consisting of a large number of bubbles, which are divided by a thin liquid film (TLF), which is made of two interacting adsorption layers. A parameter describing the stability of TLF is its thickness h, its change over time determines the drainage kinetics. The laboratory model of the mentioned situation is an air bubble, which forms TLF with the free surface of the solution. The above-mentioned model is often used when it comes to the description of more complex dispersed systems. The carried out research consisted in the analysis of the influence of an applied magnetic field on the adsorption properties of a magneto-reactive surfactant (DTAF). Additionally, our team has researched the impact of a magnetic field on the drainage of individual TLFs, formed under dynamic conditions. To achieve this aim, an apparatus has been built, its main parts are an electromagnet, a system generating a single bubble, a tensiometer, and a refractometric spectrometer. The used set-up allowed us to determine the influence of a magnetic field on the changes of the surface tension and the changes of the TLF thickness over time. As a result of the experiments, spectacular differences in the obtained values of surface tension and kinetics of foam drainage have been acquired, in the presence of a magnetic field and its absence. Foam films interacting with a magnetic field were characterized by a faster rate of drainage, the bubble itself – with a shorter lifetime. The most probable theoretical justification of the observed effects lies in the field of magnetohydrodynamics and generations of magnetic pressure.

The research was carried out thanks to the financial support of the National Science Center (NCN) as a part of the OPUS project (2017/25/B/ST8/01247).

Poster N° 9

Macroion Conformation in Electrolyte Solution – Modelling, Experiment and Slender Body Hydrodynamics

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Macroions are an important class of compounds with properties characteristic both of polymers and charged molecules. Most commonly, macroions are studied using only experimental techniques such as dynamic light scattering (DLS), laser Doppler velocimetry (LDV) and viscosity measurements. This allows one to evaluate their molar mass distribution, the radius of gyration, the contour length, intrinsic viscosity and sedimentation coefficient.

However, despite of extensive experimental research, no comprehensive characteristics of most studied macroions were acquired using simultaneously theoretical modelling and different experimental techniques. This results in only semiquantitative information about macroion conformation and may led to wrong conclusions about their properties.

Therefore, we have performed thorough characteristics of carrageenan, chitosan and poly(L-lysine) solutions using a combination of the all-atom molecular dynamics (MD) modelling, DLS, LDV and viscosity measurements. Our investigations yielded quantitative information about the macroion molecule properties such as its ionization degree, chain length and cross-section area under a broad range of conditions. We have shown that all studied macroions exhibit a flexible-rod shape with no sharp bending.

The obtained data allows the prediction of macroion adsorption kinetics and facilitate a proper interpretation of experimental techniques that require calibration, especially quartz crystal microbalance or the streaming potential measurements.

Poster Nº 10

Modeling cellular spreading and motility on curved surfaces

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Cells often adhere and migrate on curved surfaces, such as the fibers of the extra-cellular matrix (ECM), cylindrical protrusions of other cells etc. However, most of the cell biological studies examine cell migration mechanisms using cells on flat surfaces. We study the spreading and migration of a cell-like vesicle on curved surfaces, such as cylinders, sinusoidal surface etc. The vesicle is composed of curvature-sensitive proteins, that diffuse on its surface, and also recruit actin polymerization, which applies an active protrusive force. We note that on the outside of a cylinder, the vesicle coils or migrates circumferentially, rather than axially. For a cylinder of smaller radius, however, they prefer not to coil or migrate, but spreads weakly. In contrast, inside a cylinder, the vesicle prefers to elongate or migrate along the axial direction. On a sinusoidal surface with alternating dips (minima) and peaks (maxima), the vesicle behaves in similar way as inside and outside of a cylinder, respectively. The vesicle prefers to stay in the dip and align axially. However, if placed on the peak, it prefers to slide down to the dip. While migrating from one dip to another, it crosses the peak at higher angle and larger speed. Our results are in agreement with experiments, and offer an explanation for some of the observed curvature-sensitivity of cell migration patterns.

Poster N° 11

Monte Carlo simulation of particle segregation in evaporating bi-dispersed colloidal droplets

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Colloidal droplets are used in a variety of practical applications. Some applications require particles of different sizes. These include medical diagnostic methods, the creation of photonic crystals, the formation of supraparticles, and the production of membranes for biotechnology. Series of experiments have previously shown the possibility of particle separation by their size near the contact line. A mathematical model has been developed to describe this process. Bi-dispersed colloidal droplets evaporating on a hydrophilic substrate are taken into consideration. A particle monolayer is formed due to the small value of the contact angle near the periphery of such droplets. The shape of the resulting sediment is associated with the coffee ring effect. The model takes into account the particle diffusion and transfer with a capillary flow caused by liquid evaporation. Monte Carlo simulation of particle dynamics has been performed at several values of the solution concentration. The numerical results agree with the experimental observations, in which small particles accumulate closer toward the contact line than large particles.

Poster N° 12

On dispersionless transport in washboard potentials

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Phenomena of Brownian particle transport and diffusion in tilted periodic potentials are realized in many diverse systems. Superionic conductors, magnetic ratchets, optical lattices, charge-density waves, granular gases, Josephson junctions, automatic phase-lock frequency control systems are some prominent examples. These phenomena have been studied meticulously in recent decades [1]. These investigations produced a host of intriguing discoveries, including dispersionless transport. Such a coherent motion of the packet of particles formed after them leaving the initial potential well under the action of the constant bias force was reported in [2].

We reassess the "dispersionless transport regime" of Brownian particles in tilted periodic potentials. We show that the particles exhibit normal diffusive motion right after transitioning into the running state dragged by the constant bias force. No special transient dynamics appears, contrary to conjectures in the previous studies. The observed flat segment in the dispersion evolution curve is solely due to the broad spatial distribution of particles formed in the early superdiffusion stage. We quantitatively describe the whole evolution of the distribution function during superdiffusion and the transition to the normal diffusion that follows, in the framework of the 2-well potential in the velocity space model. We show that the superdiffusion exponent is $\alpha = 3$. Estimate of the duration of the ostensible "dispersionless regime" is provided. It is shown to diverge exponentially as the temperature decreases to zero.

[1] P. Hanggi, F. Marchesoni, Rev. of Mod. Phys. 81 (2009) 387.
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Poster Nº 13

Roughness spectroscopy of particle monolayers

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Surface roughness is an essential factor determining many surface phenomena, including adhesion, friction, wave reflection, microfluidics, electrochemistry, and wettability. It is conveniently described in terms of power spectral density of 2D height profile of the surface. I will discuss the power spectral density of particle monolayers widely used as sensors, substrates, catalysts, and antireflective or antimicrobial surfaces. I will demonstrate a close analogy between the surface power-spectral-density and the well known intensity of radiation scattering. I will also give a simple example of application of the function in characterizing particle monolayers

Poster N° 14

Monte Carlo simulations of liquid crystal phases: behind the scenes

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Computer simulations are a basic tool for modeling soft matter since only a handful of models can be solved exactly or they can be treated only with phenomenological theories. For most soft interactions a standard molecular dynamic (MD) integration is a go-to tool. However, hard interactions pose a problem because of infinite forces during collisions. While there exist collision event driven extensions to MD, the most straightforward way of simulating hard-core systems is the Monte Carlo Metropolis-Hasting algorithm. Although the basic version of the Monte-Carlo (MC) algorithm is easy to implement, it becomes very inefficient for a large number of interaction centers. This work summarizes some optimizations, including neighbor grid and parallelization using domain division which enable to simulate tens of thousands of interaction centers for tens of millions of full MC cycles within a reasonable time. Moreover, it provides a summary of problems that may hinder the equilibration of the system together with possible solutions to them.

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