

# BOOK OF ABSTRACTS











on Statistical Physics

**Soft Matter, Information Processing and Nonequilibrium Fluctuations** 

24 - 28 SEPTEMBER, 2023, KRAKÓW, POLAND

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

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24-28 SEPTEMBER, 2023, KRAKÓW, POLAND

September 27<sup>th</sup>, Kraków, Poland

## Mini Colloquium

in celebration of prof. Lech Longa's 70<sup>th</sup> birthday and appreciation of his numerous contributions to the understanding of liquid crystalline phases and related phenomena.



#### **Invited Speakers**

David Allender (USA)

Ewa **Górecka** (Poland)

Alberta Ferrarini (Italy)

Fernando Oliveira (Brasil)

Mikhail Osipov (UK)

Holger Stark (Germany)

Hans-Rainer **Trebin** (Germany)

Slobodan **Žumer** (Slovenia)

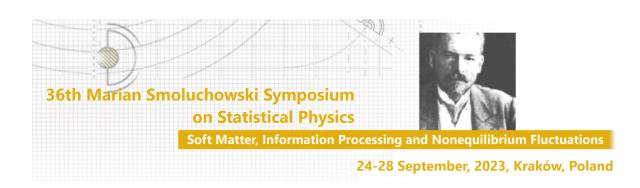
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# 36<sup>th</sup> Marian Smoluchowski Symposium on Statistical Physics 24 - 28 September, 2023, Kraków, Poland

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## **Programme**

## **Sunday 24/09**

15:00 - 15:50		Registration 🧨	
15:50 - 16:00		Welcome Address 😩	
Session 1		Chairman: Ewa Gudowska-Nowak	
16:00 - 16:40	IT	The cost of stochastic resetting	Martin Evans
16:40 - 17:05	СТ	Diffusion with time changing Hurst exponent	Jakub Ślęzak
17:05 - 17:30	СТ	Non-equilibrium criticality in the synchronization of lattices of self-sustained oscillators	Ricardo Gutiérrez
17:30 - 20:00		Get Together	

IT Invited Talk CT Contributed Talk

## Monday 25/09

Session 2		Chairman: Igor Sokolov	
09:00 - 09:40	IT	A quantum thermodynamics approach to optimization in complex systems	Alberto Imparato
09:40 - 10:05	СТ	Numerical simulation of Kibble-Zurek mechanism with Landau-Ginzburg dynamics	Fumika Suzuki
10:05 - 10:30	СТ	Many-body localization and the thermodynamic limit	Jakub Zakrzewski
10:30 - 11:00		Coffee Break 👤	
Session 3		Chairman: Martin Evans	
11:00 - 11:40	ΙΤ	Linear and nonlinear fluctuation-response relations in non-equilibrium systems - spiking neurons, stochastic oscillators, and particles in an active bath	Benjamin Lindner
11:40 - 12:05	СТ	Quantifying activity in chemically active systems with a stochastic Poisson field theory	Joël Mabillard
12:05 - 12:30	СТ	Self-organization without self-attraction in quorum-sensing active matter: the interplay between nonreciprocity and motility	Benoît Mahault
12:30 - 14:00		Lunch Break 🍴	
Session 4		Chairman: Piotr Garbaczewski	
14:00 - 14:40	IT	Generation of rare events in stochastic systems	Raúl Toral
14:40 - 15:05	СТ	Catalytically optimized search strategy	Yann Lanoiselée
15:05 - 15:30	СТ	Controlling uncertainty of empirical first-passage times in the small-sample regime	Rick Bebon
15:30 - 16:00		Coffee Break 👤	
Session 5		Chairman: Raúl Toral	
16:00 - 16:40	IT	Machine learning on uncontrolled hardware	Juan Pablo Carbajal
16:40 - 17:05	СТ	Noise management in machine learning	Karol Capała
17:05 - 17:30	СТ	Coarse-grained description of stochastic dynamics and field theoretic models for complex systems	Shankar Prasad Das
		IT Invited Talk CT C	ontributed Talk

## Tuesday 26/09

Session 6		Chairman: Juan Pablo Carbajal	
09:00 - 09:40	IT	Mean field theory of memristive systems and nanowires	Francesco Caravelli
09:40 - 10:05	СТ	Stochastic resonance in memristors	Paweł F. Góra
10:05 - 10:30	СТ	Global in time existence theorem for the full revised Enskog equation	Jacek Polewczak
10:30 - 11:00		Coffee Break 👤	
Session 7		Chairman: Aljaž Godec	
11:00 - 11:25	СТ	Binary mixtures of driven Brownian hard spheres in periodic potentials in one dimension	Artem Ryabov
11:25 - 11:50	СТ	Ensemble dependence of the critical behavior of a system with long range interaction and quenched randomness	Nir Schreiber
11:50 - 12:15	СТ	Ensemble dependence of information-theoretic contributions to the entropy production	Krzysztof Ptaszyński
12:30 - 14:00		Lunch Break 🍴	
Session 8		Chairman: Paweł F. Góra	
14:00 - 14:40	IT	Thermal relaxation asymmetry in reversible and driven systems	Aljaž Godec
14:40 - 15:05	СТ	Negative heat generation in a non-Markovian bath	Félix Ginot
15:05 - 15:30	СТ	Optimal work protocols in non-Markovian baths	Samuel Monter
15:30 - 16:00	IT	Human and viral ion channels and membranes	Andrzej Fuliński
16:00 - 16:30		Coffee Break 👤	
16:30 - 18:00		Poster Session	

## Wednesday 27/09 Prof. Lech Longa's *mini colloquium* – 70<sup>th</sup> birthday anniversary

08:45 - 09:00		Opening Speech 🚢	
Session 9		Chairman: Michał Cieśla	
09:00 - 09:40	IT	Entropic stabilization of quasicrystals	Hans-Rainer Trebin
09:40 - 10:20	IT	Universal scaling relation for growth phenomena	Fernando Oliveira
10:20 - 10:50		Coffee Break 👤	
Session 10		Chairman: Alberta Ferrarini	
10:50 - 11:30	IT	A tribute to Lech Longa: Devoting more than forty years to probing new phenomena in nematic liquid crystals	David Allender
11:30 - 12:10	IT	Theoretical models for the nematic twist-bend phase and the seminal contribution of Prof. Longa	Mikhail Osipov
12:10 - 12:50	IT	Topological constraints of activity-driven transitions from stationary defect dynamics to nematic turbulence	Slobodan Žumer
12:50 - 13:30	IT	Complex helical smectic phases made of achiral molecules	Ewa Górecka
13:30 - 15:00		Lunch Break 🎢	
Session 11		Chairman: David Allender	
15:00 - 15:40	IT	Some open questions in the elasticity of nematic liquid crystals: insights from microscopic theory	Alberta Ferrarini
15:40 - 16:20	IT	Nematic ordering in active systems	Holger Stark
16:20 - 16:45	СТ	A self-consistent mean field model for hard ellipsoids	Peter Palffy-Muhoray
16:45 - 17:15		Coffee Break 👤	
Session 12		Chairman: Wojciech Tomczyk	
17:15 - 17:40	СТ	Entropy-driven formation of modulated and frustrated mesophases in a system composed of bent-core molecules	Piotr Kubala
17:40 - 18:05	СТ	Properly dealing with recent discoveries in suspensions of bent colloidal rods by means of a grand-canonical Landau-de Gennes theory	Carmine Anzivino
18:30		Gala Dinner 🛊	
		IT Invited Talk CT	Contributed Talk

## Thursday 28/09

Session 13		Chairman: Arkady Pikovsky	
09:00 - 09:25	СТ	Mitosis of life aims in Poland 2012-2016	Krzysztof Kułakowski
09:25 - 09:50	СТ	Reentrant phase transition in the TASEP with parking spots	Valentin Anfray
09:50 - 10:15	СТ	Nonconservative diffusion processes	Piotr Garbaczewski
10:15 - 10:45		Coffee Break 👤	
Session 14		Chairman: Krzysztof Kułakowski	
10:45 - 11:25	IT	Random walks in correlated diffusivity landscapes	Igor Sokolov
11:25 - 11:50	СТ	Statisitical properties of random advection-diffusion	Arkady Pikovsky
11:50 - 12:15	СТ	Dynamical phase transition in the fluctuations of occupation fraction of $N$ non-crossing Brownian particles	Soheli Mukherjee
12:15 - 13:45		Lunch Break 🍴	

IT Invited Talk CT Contributed Talk

24 - 28 SEPTEMBER, 2023, KRAKÓW, POLAND

#### General Information

#### Venue

The conference will be held at the Faculty of Physics, Astronomy and Applied Computer Science of the Jagiellonian University, ul. Łojasiewicza 11 (lecture hall A1-03, 1<sup>st</sup> floor), which is about 30/40-minute ride from the city center. One can get there using the public transportation (trams number 17, 18, 52, 62 or bus number 578 and 662) to reach "Norymberska" (or "Ruczaj") stop and then by taking a short walk (see page 10). Note that the direction of tram/bus (final station) should be "Czerwone Maki P+R".

- Tram 17, 18, 52 and 62 run through the city center.
- Tram 18 is reachable within the vicinity of Royal Castle Wawel.
- Bus 578 and 662 are reachable within the outskirts of so-called "Old Town" (Stare Miasto).

#### Registration

Conference desk will be located in the main hall (building A, ground floor) of the Faculty of Physics, Astronomy and Applied Computer Science (see page 10). Registration will be open from 15:00 to 15:50 on Sunday 24/09. On the other days please consult Symposium organizers, designated by special badges, in order to complete registration.

#### **Invited & Contributed talks**

Talks will be given in the lecture hall A1-03 (1<sup>st</sup> floor). It is advisable to use locally available computer (with Windows operating system) for the presentation (either in pdf or ppt(x) format). You can alternatively use your personal laptop, but you are kindly asked to check at least one session before your talk if all details of your file are properly projected onto the screen. Please use preferentially coffee breaks or lunch for this check and for uploading the files to the local computer. Symposium organizers will provide you with technical support.

Invited talks are scheduled for 40 min. (35 min. + 5 min. Q&A), while contributed talks are scheduled for 25 min. (20 min. + 5 min. Q&A). Chair persons will be instructed to follow the time schedule rigorously

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## General Information (continued)

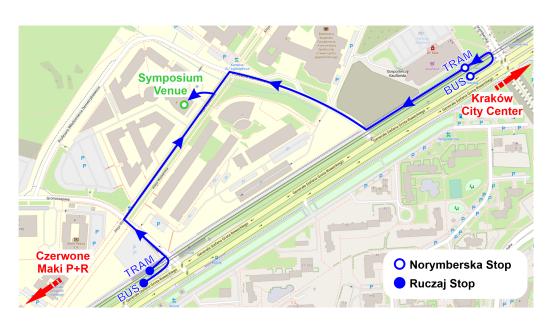
#### Poster session

The Poster session is scheduled for Tuesday 26/09 at 16:30. Cork boards will be available: 120 cm x 90 cm (maximum paper size standard is A0) and pins to fix the posters. Please check the "Posters" section to find out the number assigned to your poster. After the Poster session, posters that have not been dismounted before the lunch on Thursday will be removed by the Organizers.

#### Internet access

Access via Eduroam and local Wi-Fi network will be available during the Symposium.

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#### Presentations (continued)

Sunday 24/09, 16:00 - 16:40

## The cost of stochastic resetting IT

Martin Evans<sup>1,\*</sup>, John C. Sunil<sup>1</sup>, Richard A. Blythe<sup>1</sup> and Satya N. Majumdar<sup>2</sup>

- <sup>1</sup> SUPA, School of Physics and Astronomy, University of Edinburgh, Peter Guthrie Tait Road, Edinburgh EH9 3FD, UK
- <sup>2</sup> Université Paris-Saclay, CNRS, LPTMS, 91405, Orsay, France

Resetting a stochastic process has been shown to expedite the completion time of some complex tasks, such as finding a target for the first time. In this talk we consider the cost of resetting by associating a cost to each reset, which is a function of the distance travelled during the reset event. We show some unexpected results. First, in the limit of a vanishing resetting rate, the mean total cost is finite for a linear cost function and diverges for a super-linear cost function. This result contrasts with the case of no resetting where the cost is always zero. Second, the resetting rate that minimises the time to completion, including the total resetting cost, is reduced from the case of no cost for a linear cost function, remains unchanged for a quadratic cost function but may be increased for a super-quadratic cost function. In the latter case an increased rate of resetting reduces the chance of costly resets.

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#### Presentations (continued)

Sunday 24/09, 16:40 - 17:05

### Diffusion with time changing Hurst exponent CT

<u>Jakub Ślęzak</u>1,\* and Ralf Metzler<sup>2,3</sup>

- <sup>1</sup> Hugo Steinhaus Center, Wrocław University of Science and Technology, Wrocław, Poland
- <sup>2</sup> Institute of Physics & Astronomy, University of Potsdam, Potsdam, Germany
- <sup>3</sup> Asia Pacific Centre for Theoretical Physics, Pohang 37673, Republic of Korea

Strong symmetries of Fractional Brownian Motion (FBM) make its Hurst index H the unifying number governing both its short (fractal dimension 2-H) and long time (mean squared displacement  $\propto t^{2H}$ ) properties. This fact restricts some of its applications-crucially it makes it impossible to describe an increasing number of regime switching anomalous diffusion systems in which the anomalous diffusion exponent and the diffusivity change as functions of time. These are, e.g., motions of a tracer in the changing viscoelastic environment of cells during their cycle, solutions under pressure and/or concentration changes, the motion of lipid molecules in cooling bilayer membranes or passive and active intracellular movement after treatment with chemicals. In order to overcome the limitations of FBM, multifractional Brownian motion (MFBM) models were created, initially motivated by terrain modelling. However, most of the existing types of MFBM use Hurst index as purely local measure of the path roughness and cannot be used as models of physical diffusion switching from one type of complex environment to another.

We will show how to overcome this limitation and present models of a particle diffusing in a complex environment for which conditions change in time and after the transition new displacements are governed by a new diffusivity and a new Hurst exponent while also keeping the memory of its history before the transition. We can describe both smooth and stepwise transitions. We obtain the mean squared displacement and correlations of these models and study their behaviour. Finally, we present estimation methods and discuss how this modelling approach can help with analysing experimental data.

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#### Presentations (continued)

Sunday 24/09, 17:05 - 17:30

# Non-equilibrium criticality in the synchronization of lattices of self-sustained oscillators CT

Ricardo Gutiérrez<sup>1,\*</sup> and Rodolfo Cuerno<sup>1</sup>

<sup>1</sup> Complex Systems Interdisciplinary Group, Department of Mathematics, Universidad Carlos III de Madrid (Spain)

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The study of synchronous dynamics has traditionally focused on the identification of threshold parameter values for the transition to synchronization, and on the nature of such transition. The dynamical process whereby systems of self-sustained oscillators synchronize, however, has been much less studied. While one might reasonably expect such a process to be strongly system-dependent, in Ref. [1] we have recently shown that indeed it contains some robust universal features, which originate in a mathematical connection existing between synchronization models and the equations of surface growth processes. By means of a detailed numerical study of one-dimensional systems of phase oscillators and several limit-cycle oscillators, we provide evidence indicating that the synchronization process in these systems is characterized by forms of generic scale invariance associated with the universality classes of kinetically rough interfaces with columnar disorder. Moreover, the phase fluctuations around the average growth follow a ubiquitous Tracy-Widom probability distribution, which is frequently associated with the Kardar-Parisi-Zhang nonlinearity. Synchronization and surface growth processes thus seem to be much more closely related than previously anticipated.

#### References

[1] R. Gutiérrez and R. Cuerno, Phys. Rev. Research 5, 023047 (2023).

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#### Presentations (continued)

Monday 25/09, 09:00 - 09:40

## A quantum thermodynamics approach to optimization in complex systems

Alberto Imparato<sup>1,\*</sup>

<sup>1</sup> Department of Physics and Astronomy, University of Aarhus, Ny Munkegade, Building 1520, DK–8000 Aarhus C, Denmark

An optimization problem can be translated into physics language as the quest for the energy minimum of a complex system with a Hamiltonian that encodes the problem itself. Stretching the analogy further, the optimization problem can be seen as the controlled cooling of such a complex system so as it lands in a minimum of its complex energy landscape corresponding to the optimal solution of the given problem. I will introduce and discuss two methods for quantum cooling, and thus for optimization, entailing the use of quantum, non-Markovian baths connected to the system of interest. In the first method the bath is prepared in a suitable low energy initial state that efficiently cools down the system of interest. In the second method the bath is measured, and post-measurement excited states of the bath are selected, that correspond to low energy states for the system of interest.

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### Presentations (continued)

Monday 25/09, 09:40 - 10:05

# Numerical simulation of Kibble-Zurek mechanism with Landau-Ginzburg dynamics CT

Fumika Suzuki<sup>1,2,3,\*</sup>

- <sup>1</sup> ISTA (Institute of Science and Technology Austria), Am Campus 1, 3400 Klosterneuburg, Austria
- <sup>2</sup> Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA
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The Kibble-Zurek mechanism (KZM) is a theoretical framework that describes the dynamics of non-equilibrium processes and defect formation in systems undergoing second-order phase transitions. This mechanism finds widespread application in various fields, including cosmology and condensed matter physics.

I will explore the numerical simulation of KZM using Landau-Ginzburg dynamics and its potential applications in superconducting phase transitions involving intrinsic fluctuating magnetic fields and the miscible-immiscible phase transition of Bose-Einstein condensates.

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#### Presentations (continued)

Monday 25/09, 10:05 – 10:30

#### Many-body localization and the thermodynamic limit CT

Jakub Zakrzewski<sup>1,2,\*</sup>

<sup>1</sup> Institute of Theoretical Physics, Jagiellonian University, Łojasiewicza 11, 30-348 Kraków, Poland

Many-body localization (MBL) seems to be a robust example of ergodicity breaking. While manifested in small systems and for short times (in experiment) its very existence in the thermodynamic limit has been questioned recently. I will discuss recent efforts to answer this query by various means from exact diagonalization to large systems dynamics using tensor network approaches, the role of symmetries and conservation laws. Different types of disorder will be discussed as well as systems without disorder (if time permits). The talk is based on several recent papers, notably PRB 105, 224203 (2022) and PRB 107, 115132 (2023).

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#### Presentations (continued)

Monday 25/09, 11:00 - 11:40

# Linear and nonlinear fluctuation-response relations in non-equilibrium systems - spiking neurons, stochastic oscillators, and particles in an active bath

Benjamin Lindner<sup>1,2,\*</sup>

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The fluctuations and the response of stochastic systems are not independent but related by fluctuation-dissipation theorems or, equivalently, fluctuation-response relations (FRRs). Originally introduced for systems in thermodynamic equilibrium, generalizations of such relations for non-equilibrium situations have been discussed since the 1970's and are particularly appealing for biological systems. FRRs are useful to (i) prove that a system is outside of equilibrium, (ii) prove that it does not follow Markovian dynamics, (iii) extract parameters and statistics of intrinsic noise sources, (iv) derive analytically statistics of nonlinear stochastic models. In my talk I report progress on several FRRs in systems far from equilibrium. I discuss a nonlinear FRR for systems that can be perturbed by a step stimulus, which can be used as an efficient test of Markovianity. I present a universal description for stochastic oscillators, that results in a simple FRR in terms of a new complex-valued transform of the original oscillator variables. Most importantly, I derive a new class of FRRs for spiking neurons that relate the pronounced fluctuations of spontaneous neural firing to their average response to sensory stimuli, i.e. to the processing of sensory information that is the *raison d'etre* of neural systems [1-3].

#### References

- [1]. B. Lindner, Phys. Rev. Lett. 129, 198101 (2022).
- [2] A. Perez-Cervera, B. Gutkin, P. J. Thomas, and B. Lindner, *PNAS*, accepted (2023).
- [3] K. Engbring, D. Boriskovsky, Y. Roichman, and B. Lindner, *Phys. Rev. X* 13, 021034 (2023).

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### Presentations (continued)

Monday 25/09, 11:40 - 12:05

## Quantifying activity in chemically active systems with a stochastic Poisson field theory CT

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Chemically active systems are characterized by the presence of chemical processes which convert energy from the environment to perform activity. Examples are self-propelled particles, active droplets, active gels or molecular motors. The continuous flow of energy, stemming from the chemical reactions, prevents the system to reach thermal equilibrium at molecular scales. For this reason, active matter is known to be intrinsically out of equilibrium. A precise understanding of the non-equilibrium character of active matter remains however a puzzling question. Recent observations in living cells, which are typical examples of active systems in biophysics, even suggest that the local-equilibrium approximation might hold on the spatiotemporal scales related to the formation of condensates.

In this presentation, a framework to quantify activity using fluctuations of heat in the system is introduced [1]. The origin of these fluctuations is of two kinds, either stemming from the active processes or related to the passive thermal fluctuations. The formulation of a field theory with stochastic fluctuating noise and Poisson statistics makes it possible to describe the fluctuations arising from activity. Passive fluctuations, related to the stochasticity in the heat transport at local equilibrium, are described by a stochastic field theory with Gaussian white noise. The dominant contribution in the heat fluctuation provides an indication of the non-equilibrium character of the system. For the length and time scales where the passive thermal fluctuations are dominant, the system might be well approximated by local thermal equilibrium and the relative importance of passive versus active contribution provides a way to quantify the activity.

#### References

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### Presentations (continued)

Monday 25/09, 12:05 - 12:30

# Self-organization without self-attraction in quorum-sensing active matter: the interplay between nonreciprocity and motility CT

Benoît Mahault<sup>1,\*</sup>, Jaime Agudo-Canalejo<sup>1</sup>, Ramin Golestanian<sup>1</sup> and Yu Duan<sup>1</sup>

Over the past years, the generation of interactions breaking action-reaction symmetry has emerged as new paradigm for active matter. Such nonreciprocal interactions have in particular been argued to constitute a generic route for the emergence of steady states breaking time reversal symmetry. The generalization of the Cahn-Hilliard theory of phase separation to nonreciprocal mixtures predicts, for example, the emergence of traveling states when intra-species attraction leads to demixing while chasing inter-species interactions are present. Here, we study a minimal model of active phase separation involving two species of particles regulating their self-propulsion speed via quorum-sensing rules. Combining simulations of the microscopic model and linear stability analysis of the associated coarse-grained field theory, we identify a mechanism for dynamical pattern formation that does not rely on the standard route of intraspecies effective attractive interactions. Instead, our results reveal a highly dynamical phase of chasing bands induced only by the combined effects of self-propulsion and nonreciprocity in the inter-species couplings. Turning on self-attraction, we find that the system may phase separate into a macroscopic domain of such chaotic chasing bands coexisting with a dilute gas. We show that the chaotic dynamics of bands at the interfaces of this phase-separated phase results in anomalously slow coarsening.

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#### Presentations (continued)

Monday 25/09, 14:00 - 14:40

## Generation of rare events in stochastic systems

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Rare events, although infrequently occurring, can have significant consequences in various fields such as epidemics, ecological dynamics, biological switches, chemical reactions, and natural disasters. Existing techniques like the Wentzel-Kramers-Brillouin (WKB) method and transition path sampling algorithms provide insights into rare event paths, but they have limitations. The WKB method only provides information about the most likely path, while transition path sampling methods require detailed balance and forward flux algorithms may produce statistically biased trajectories. Here I will consider the use of "stochastic bridges" to analyze the statistics of rare trajectories. Stochastic bridges are paths that pass through specified start and end points, and they have been utilized in various fields such as physics, finance, and information processing. I will show that the statistics of the target stochastic process can be obtained by associating a statistical weight with each stochastic bridge, enabling dedicated computational effort towards rare trajectories without introducing bias or interdependence. The proposed method for bridge generation is flexible and applicable to general target processes, without requiring detailed balance, small-noise approximation, or the introduction of artificial parameters like temperatures. The stochastic bridges produced capture the full statistics of the ensemble of transition paths between long-lived states, allowing for the sampling of fluctuations around the WKB instanton. This enables the assessment of the accuracy of the WKB approximation scheme at different levels of noise. I will show specific examples, such as extinction trajectories of a Susceptible-Infected-Susceptible model in the endemic regime, the distribution of first-passage times in a biased random walk, and noise-driven transitions from undifferentiated to differentiated cell states in a cell differentiation model. These analyses provide further insights into the dynamics and statistics of rare events in different systems.

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#### Presentations (continued)

Monday 25/09, 14:40 - 15:05

## Catalytically optimized search strategy CT

<u>Yann Lanoiselée</u><sup>1,2,\*</sup>, Jak Grimes<sup>1,2</sup>, Zsombor Koszegi<sup>1,2</sup>, Tamara Miljus<sup>1,2</sup>, Shannon L. O'Brien<sup>1,2</sup>, Tomasz M. Stepniewski<sup>3</sup>, Brian Medel-Lacruz<sup>3</sup>, Mithu Baidya<sup>4</sup>, Maria Makarova<sup>1,2,5</sup>, Ravi Mistry<sup>1,2</sup>, Joëlle Goulding<sup>2,6</sup>, Julia Drube<sup>7</sup>, Carsten Hoffmann<sup>7</sup>, Dylan M. Owen<sup>2,8</sup>, Arun K. Shukla<sup>4</sup>, Jana Selent<sup>3</sup>, Stephen J. Hill<sup>2,6</sup> and Davide Calebiro<sup>1,2</sup>

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Understanding how information is transmitted from the exterior to the interior of living cells is essential for developing new therapeutic strategies. Despite recent structural advances, the mechanisms that govern interactions of membrane-bound receptors with intracellular arrestin molecules at the plasma membrane remain elusive. Here [1], we combine single-molecule microscopy with molecular dynamics simulations to dissect the complex sequence of events involved in b-arrestin interactions with both receptors and the lipid bilayer.

We carefully characterize the spatiotemporal co-dynamics of receptors and arrestins. We show that receptor and arrestin diffusion has multiple states that are linked to biological function.

Unexpectedly, our results reveal that b-arrestin spontaneously inserts into the lipid bilayer and transiently interacts with receptors via lateral diffusion on the plasma membrane. Moreover, they indicate that following receptor interaction, the plasma membrane stabilizes b-arrestin in a longer-lived membrane-bound state, allowing it to diffuse to clathrin-coated pits separately from the activating receptor.

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## Presentations (continued)

This constitutes a new mechanism for the target-search strategy that combines surfacemediated diffusion with catalytic activation.

These results open the way to new questions in search strategies and expand our current understanding of b-arrestin function at the plasma membrane.

#### References

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#### Presentations (continued)

Monday 25/09, 15:05 – 15:30

# Controlling uncertainty of empirical first-passage times in the small-sample regime CT

Rick Bebon<sup>1,\*</sup> and Aljaž Godec<sup>1</sup>

First-passage phenomena are ubiquitous in nature and at the heart of e.g., reaction kinetics, gene regulation, the foraging behavior of animals, and stock option dynamics. Whereas theoretical studies focus on predicting statistics of the first-passage time for a given process, practical applications typically aim at inferring kinetic rates, i.e. inverse mean first-passage times, from experimental or simulation data. The inference of such empirical first-passage times is however challenging because usually, only a small number of realizations are available, giving rise to high uncertainties and non-Gaussian errors.

We present general bounds on the probability that the empirical first-passage time inferred from a sample of n independent realizations deviates from the true mean first-passage time by more than any given amount in either direction. We construct non-asymptotic confidence intervals that hold in the elusive small-sample regime and thus fill the gap between asymptotic methods and the Bayesian approach that is known to be sensitive to prior belief and tends to underestimate uncertainty in the small-sample setting. Our results allow for model-free error control and reliable error estimation in kinetic inference, and are thus important for the analysis of experimental and simulation data in the presence of limited sampling.

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#### Presentations (continued)

Monday 25/09, 16:00 - 16:40

### Machine learning on uncontrolled hardware

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Many machine learning (ML) algorithms require complete knowledge of the hardware in which they run. They also require detailed control of the hardware physical properties. Reservoir Computing (RC) is a ML algorithm that can be implemented with minimal control of the physical properties of the hardware. In RC, a non-linear dynamical system acts as a generator of an infinite features dictionary, which is fed into a liner regression layer. The former is the only component that needs to be tuned for learning. This algorithm excels at processing information generated by dynamical systems using observed time-series data. It requires very small training data sets, uses linear optimization, and thus requires minimal computing resources.

The relevance of this type of algorithm is motivated by the reemergence of analog hardware as an alternative solution for specialized ML applications. In particular, neuromorphic hardware, using combination of analog and digital elements, are becoming increasingly competitive in ML applications, offering high-speed, low-footprint, and low-power solutions. In this talk I will introduce Reservoir Computing, showcase its implementation in current digital computers, and then discuss the advantages of embedding the algorithm in specialized hardware [1-3].

#### References

- [1] Carbajal et al., Neural Comput. 27(3), 725 (2015).
- [2] Caravelli & Carbajal, *Technologies* **6**(4), 118 (2018).
- [3] Gauthier et al., Nat. Commun. 12(1), 5564 (2021).

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### Presentations (continued)

Monday 25/09, 16:40 - 17:05

## Noise management in machine learning CT

Karol Capała<sup>1,\*</sup>, Varun Ravi Varma<sup>1</sup> and Jose Sousa<sup>1</sup>

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Noise can significantly impact Machine Learning performance, both in real-world data and due to adversarial attacks. Our method aims to mitigate the effect of noise by introducing data abstractions, which reduce the impact of noise but may result in some loss of information and accuracy. The poster explores various approaches to abstractions for numerical data and binary classification tasks. Experiments compare the performance of random forest, logistic regression, support vector machine and artificial neural network using raw and abstracted data. We also extensively studied the robustness to noise in the case of artificial neural network.

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### Presentations (continued)

Monday 25/09, 17:05 - 17:30

# Coarse-grained description of stochastic dynamics and field theoretic models for complex systems CT

Shankar Prasad Das1,\*

The continuum field theoretic approach to describing a many-particle system has been very useful in understanding its thermodynamic and time-dependent behaviour. Our discussion will be on the fluctuating hydrodynamic description used to study the behaviour of a system of passive systems and the active matter of self-propelled particles. The dynamics are primarily formulated in terms of a set of collective modes of the system. Starting from a set of microscopic balance equations which are exact representations of the stochastic dynamics of a many particle system, the description with smooth Spatio-temporal dependencies follow.

We demonstrate how the appearance of the self-propelling terms and the breaking of Galilean invariances in the equations for the active-matter hydrodynamics are linked to the microscopic dynamics of the individual units.

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#### Presentations (continued)

Tuesday 26/09, 09:00 - 09:40

### Mean field theory of memristive systems and nanowires **I**

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There has been a lot of interest in nanoscale devices that can mimic some brain functionalities. In this talk, we discuss mean field theoretical techniques that can be used to study nanoscale devices with memory, including recent experiments on self-organizing nanowires. A large body of work has shown that PVP-coated self-organizing Ag nanowires have a dynamic response to an applied voltage that mimics the short-term plasticity of neuronal synapses. However, while every single experiment has a different connectivity pattern, it is observed a conductance response that is not strongly dependent on the details of the nanowire network. In this talk, we use recent results on the study of memristive networks that apply to dynamical systems with constraints, such as Kirchhoff laws, to derive a mean field theory for networks of nanowires. We show how these mean field theories have potential applications that go beyond the specificity of the system, but that can be applied to a larger class of dynamical systems. We also comment on more recent use of Weingarten calculus to derive these mean field theories.

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### Presentations (continued)

Tuesday 26/09, 09:40 - 10:05

#### Stochastic resonance in memristors CT

Paweł F. Góra<sup>1,\*</sup>

Two models in which dynamic conductance is modelled as an overdamped motion in a potential, display memristive behavior and stochastic resonance when subject to an external noise. One is a tilted two-well potential and the other a monostable well but with both additive and mutiplicative noises.

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### Presentations (continued)

Tuesday 26/09, 10:05 – 10:30

## Global in time existence theorem for the full revised Enskog equation CT

Jacek Polewczak<sup>1,\*</sup>

I prove global in time existence of solutions to the full revised Enskog equation. This equation generalizes the Boltzmann theory to dense gases in two ways:

- 1. by taking into account the fact that the centers of two colliding spheres are at a distance a, equal to the diameter of hard spheres.
- 2. by increasing the collision frequency by a factor  $Y_0$  which nowadays is identified with the radial pair correlation function  $g_2$  for the system of hard spheres at a uniform equilibrium.

In contrast to the dilute gas mode described by the Boltzmann equation, the Enskog equation includes spatial pair correlation function for hard-spheres potential and depends in a highly non linear way on the local density of dense gas. The full revised Enskog equation refers to the case where  $g_2$ , the pair the correlation function (for non-uniform equilibrium of hard-spheres) is in general form. In terms of the virial expansion (in local density n, spatially dependent) at contact value,  $g_2$  reads:

$$q_2(n) = 1 + V_1(n) + V_2(n) + \dots + V_N(n) + \dots$$

where the term  $V_1(n)$  depends on n linearly,  $V_2(n)$  depends on n quadratically,  $V_N(n)$  depends on n as  $n^N$ , and so on.

Circa 30 years ago Arkeryd-Cercignani proved the result for the truncated  $g_2$ , i.e., when  $g_2=1$  (no density dependence). The case with  $g_2=1$  refers to the so called Boltzmann-Enskog equation. It differs from the Boltzmann equation only by existence of the shifts in the spatial variable in the collisional integral.

Since then many researchers tried/wanted to prove the result for general form of  $g_2$ . Dependence of  $g_2$  on n requires a different approach and new tools, as compared to Arkeryd-Cercignani proof ([1]). Additionally, this result finally completes and fulfills the existence result for the revised Enskog Equation.

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## Presentations (continued)

The proof of existence of solutions to the revised Enskog equation is based on two constructions:

- 1. Construction of an H-functional (see [2]), where the full expansion of  $g_2$  is used, but convergence of the series was not addressed.
- 2. Construction of a special sequence of stochastic kinetic equations (studied in [3]) and the proof that their solutions converge to weak solutions of the revised Enskog equation.

#### References

- [1] L. Arkeryd and C. Cercignani, J. Stat. Phys. **59**, 845-867 (1990).
- [2] M. Mareschal, J. Bławzdziewicz, and J. Piasecki, Phys. Rev. Lett. 52, 1169-1172 (1984).
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#### Presentations (continued)

Tuesday 26/09, 11:00 - 11:25

## Binary mixtures of driven Brownian hard spheres in periodic potentials in one dimension CT

Artem Ryabov<sup>1,\*</sup>, David Voráč<sup>1</sup> and Philipp Maass<sup>2</sup>

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We discuss the impact of polydispersity on particle currents generated by Brownian hard spheres when they are driven through periodic potentials by a constant drag force. Considering random mixtures of two types of spheres, we explain the variation of the currents with the mixing ratio of the two components and with the hard-sphere diameters. A basic unit cell exists in the space of the two hard sphere diameters. Knowing the behavior of observables in the basic unit cell yields their behavior for arbitrary values of the diameters. The underlying mapping of observables explains repeating features in the dependence of currents on the particle size. The overall variation of particle currents with the mixing ratio and hard sphere diameters is reflected by their variation in the limit where the system is fully covered by hard spheres. In this limit, the currents can be predicted analytically. Our analysis explains the occurrence of pronounced maxima and minima of the currents by changes of an effective potential barrier for the center-of-mass motion.

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### Presentations (continued)

Tuesday 26/09, 11:25 - 11:50

## Ensemble dependence of the critical behavior of a system with long range interaction and quenched randomness CT

Nir Schreiber<sup>1,\*</sup>, Reuven Cohen<sup>1</sup> and Simi Haber<sup>1</sup>

A system with long range interaction (LRI) is usually characterized by a non-extensive energy. While, by properly scaling the Hamiltonian of the system, the energy can become extensive, it may still suffer from non-additivity. In other words, such a system with volume V and (rescaled) energy E, cannot be divided into two subsystems with energies  $E_1, E_2$ , where  $E = E_1 + E_2 + o(V)$ .

A system is expected to have equivalent thermodynamics within the canonical and the microcanonical ensembles, provided that its energy is additive. Conversely, non-additivity of the energy may result in peculiar microcanonical phenomena (that are not observed in the canonical ensemble) such as negative specific heat or the presence of microstates that are inaccessible to the system, leading to breaking of ergodicity.

The Blume-Emery-Griffiths (BEG) model with mean-field-like interaction is a simple example of a model with LRI. We employ that model to propose a mechanism which leads to an inequivalence of the two ensembles, without interfering with the interaction content. To be more specific, we consider a hybrid system governed by the BEG Hamiltonian, where the spins are randomly quenched such that some of them are "pure" Ising and the others admit the BEG set of states. It is found, by varying the concentration of the Ising spins while keeping the parameters of the Hamiltonian fixed, that the model displays different canonical and microcanonical phase portraits in concentration-temperature space. Phenomenological indications that these portraits are rich and rather unusual are found.

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### Presentations (continued)

Tuesday 26/09, 11:50 - 12:15

## Ensemble dependence of information-theoretic contributions to the entropy production CT

Krzysztof Ptaszyński<sup>1,\*</sup> and Massimiliano Esposito<sup>2</sup>

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The entropy production of an open system coupled to a reservoir initialized in a canonical state can be expressed as a sum of two microscopic information-theoretic contributions: the system-bath mutual information and the relative entropy measuring the displacement of the environment from equilibrium. We investigate whether this result can be generalized to situations where the reservoir is initialized in a microcanonical or in a certain pure state (e.g., an eigenstate of a nonintegrable system), such that the reduced dynamics and thermodynamics of the system are the same as for the thermal bath. We show that while in such a case the entropy production can still be expressed as a sum of the mutual information between the system and the bath and a properly redefined displacement term, the relative weight of those contributions depends on the initial state of the reservoir. In other words, different statistical ensembles for the environment predicting the same reduced dynamics for the system give rise to the same total entropy production but to different information-theoretic contributions to the entropy production.

#### References

[1] K. Ptaszyński and M. Esposito, *Phys. Rev. E* 107, L052102 (2023).

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### Presentations (continued)

Tuesday 26/09, 14:00 - 14:40

## Thermal relaxation asymmetry in reversible and driven systems

Aljaž Godec1,\*

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According to conventional wisdom, a macroscopic system placed in an environment with a different temperature relaxes to the temperature of the surroundings, mediated by the flow of heat that is set only by the instantaneous temperature difference. However, when rapid changes in temperature push a system far from thermodynamic equilibrium, thermal relaxation becomes asymmetric. That is, under quite general conditions heating is in fact faster than cooling. In the talk I will introduce and explain the relaxation asymmetry in reversible as well as detailed-balance violating systems, thereby highlighting that noisy systems do not relax by passing through local equilibria.

- [1] A. Lapolla & AG, Phys. Rev. Lett. 125, 110602 (2020).
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- [3] C. Dieball, G. Wellecke, & AG, arXiv:2304.06702 (2023).

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### Presentations (continued)

Tuesday 26/09, 14:40 - 15:05

## Negative heat generation in a non-Markovian bath CT

Félix Ginot<sup>1,\*</sup>, Clemens Bechinger<sup>1</sup> and Samuel Monter<sup>1</sup>

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Stochastic Thermodynamics usually investigates and describes Markovian systems where memory is absent. A typical example is Brownian Motion, where dynamics are overdamped with a delta-correlated noise term. Yet this Markovian hypothesis is very strong, and only valid for a limited range of time and length scales. More generally, a wide range of physical systems exhibit memory with finite relaxation times, which cannot be captured by Markovian models. Such memory effects not only derive from nonidealities, but can also be actively sought, to develop new physical properties and applications. In this work we apply stochastic Thermodynamics to a model non-Markovian bath made of a viscoelastic fluid. This complex fluid is characterized by a stress memory: energy injected in the bath is locally trapped and needs time to fully diffuse and be absorbed. In theory, this energy can be interpreted as a local excess heat which should be usable to produce deterministic work.

In our experiments, we measure the stochastic work, heat and internal energy of a colloidal particle inside a moving optical potential. We first show that the first law still applies, and that work is fully converted into heat and potential energy. Next we highlight that after applying work on the system, heat (and therefor entropy) can temporarily decrease, confirming the previous hypothesis. This negative heat is still limited by the amount of work that was initially spent into the system, and therefore doesn't violate the second law of thermodynamics. Finally, we discuss the implications of this finding and highlight some consequences for thermodynamics cycles, which could optimize such effects.

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### Presentations (continued)

Tuesday 26/09, 15:05 - 15:30

## Optimal work protocols in non-Markovian baths CT

Samuel Monter<sup>1,\*</sup>, Sarah A. M. Loos<sup>2</sup>, Félix Ginot<sup>1</sup> and Clemens Bechinger<sup>1</sup>

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Optimal protocols have been a subject of intense research in stochastic thermodynamics due to their importance for the understanding of biological processes and the operation of heat engines at the micro- and nanoscale. In this study, we experimentally investigate protocols to transport a Brownian particle over a given distance within a finite time using an optical trap that minimize the work spend on the particle. When performing such optimal protocols in viscous, i.e., Markovian baths, we find that the optimal protocol is characterized by sudden jumps of the trap position at the start and end of the protocol interconnected by a continuous linear motion. Our findings are in quantitative agreement with theoretical predictions. When performing similar experiments in a viscoelastic fluid which exhibits a relaxation time on the order of the protocol duration, pronounced differences are observed. While the still having symmetric jumps at the beginning and end, the corresponding protocol now follows a non-linear S shaped curve. Even though a point symmetric trap motion does not guarantee optimality, we find, that the averaged particle trajectories during the optimal work protocols are always point symmetric. Interestingly, this is the case both for Markovian and non-Markovian baths. Our findings do not only provide a deeper understanding of the underlying principles governing optimal protocols, but also give insight into the general characteristics of transport in non-Markovian environments.

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### Presentations (continued)

Tuesday 26/09, 15:30 - 16:00

### Human and viral ion channels and membranes IT

Andrzej Fuliński<sup>1,\*</sup> and Agata Wawrzkiewicz-Jałowiecka<sup>2</sup>

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The paper deals in the first place with the cooperation of biomembranes and bionanochannels, and then with mechanism(s) of observed experimentally Open/Closed (O/C) sequences of states of all biochannels, and with influence of external physical fields on ionic currents through viral nanochannels.

Model and simulations of the behaviour of currents in ionic nanochannels are presented in an attempt to better understand the mechanism(s) of O/C sequences, i.e., random interruptions of ionic flows observed in all known biochannels, including the viral ones, and in some synthetic nanopores. This process, though seemingly uneconomic, but observed in measurements, appears to be fixed by evolution at least as early as in cyanobacteria, i.e., ca. 10<sup>9</sup> years ago.

Furthermore, model and simulations of suggested influence of external physical fields on ionic currents through viral nanochannels will be presented.

Proposals of simple and realistic experimental verifications of this aging-O/C hypothesis, of the role of cell membrane, and of possible influence of external physical fields on the ionic currents through viral nanochannels will also be discussed.

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### Presentations (continued)

Wednesday 27/09, 09:00 - 09:40

## Entropic stabilization of quasicrystals IT

Hans-Rainer Trebin<sup>1,\*</sup>

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Among the soft matter systems one finds crystalline and liquid crystalline structures, but in the meantime also quasicrystalline. These can have fivefold or more than sixfold symmetries, which are not compatible with translational symmetry. Model structures are tesselations with more than one tile subdued to matching rules, or projections from higher dimensional periodic crystals. The higher dimension stands for the number of those reciprocal wave vectors in the spectrum, which are linearly independent over the integers. As a consequence quasicrystals possess in addition to the standard phonon (strain) degree of freedom also a phason (strain) degree of freedom. In the tiling picture the latter shows up as flips of the tile vertices. The random tiling hypothesis assumes, that the flips enlarge the configurational space, giving rise to a large entropy and making quasicrystals high temperature phases. I shall deal with the two-dimensional decagonal Tübingen triangle tiling. It can be represented as a tiling with two golden triangles or alternatively with five different polygons. There is a confusing large number of vertex environments in quasicrystals, but also an efficient book keeping tool, denoted polar calculus. It allows to determine the number of arbitrary vertex environments. We have extended it to count the number of all possible vertex flips. With vertex energies from a molecular dynamics simulation and the vertex and flips statistics from the polar calculus we could determine the phason dependent free energy and the phason elastic constants, describing the flips by an Ising and a ten states Potts model. Stability is attained by a soft phason transition only at a higher temperature, proving the random tiling hypothesis.

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### Presentations (continued)

Wednesday 27/09, 09:40 - 10:20

## Universal scaling relation for growth phenomena

<u>Fernando Oliveira</u><sup>1,2,3,\*</sup>, Thiago A. de Assis<sup>1,3</sup>, Edwin E. Mozo Luis<sup>1</sup> and Evandro A. Rodrigues<sup>1</sup>

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The Family-Vicsek relation [1] is a seminal universal relation obtained for the global roughness at the interface of two media in the growth process. In this Letter, we revisit the scaling analysis and, through both analytical and computational means, show that the Family-Vicsek relation can be generalized to a new scaling independent of the lateral size, substrate dimension d, and scaling exponents. This is part of universal behavior, since scaling [2], renormalization and fractals [3-7] are connected. We use properties of the Edwards-Wilkinson and lattice models in the Kardar-Parisi-Zhang and Villain-Lai-Das Sarma universality classes for  $1 \leqslant d \leqslant 3$  to support our claims.

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## Presentations (continued)

Wednesday 27/09, 10:50 - 11:30

## A tribute to Lech Longa: Devoting more than forty years to probing new phenomena in nematic liquid crystals

David Allender<sup>1,2,\*</sup>

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In this talk I will present my memories of a four-decade long connection, both professional and personal with Professor Lech Longa. I will focus on the primary ways this connection developed and grew: visits I made to the Jagiellonian University, visits he made to Kent State University (including a year-long Fulbright Fellowship), and two sets of biennial conferences we both attended, namely the Liquid Crystal Gordon Conference, and the International Liquid Crystal Conference. Our scientific interests intersected in many ways, but I will simplify by briefly discussing just two areas of research we contributed to: biaxiality and the search for a biaxial nematic phase, and a theoretical understanding of the now experimentally well-established twist-bend nematic phase.

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## Presentations (continued)

Wednesday 27/09, 11:30 - 12:10

## Theoretical Models for the nematic twist-bend phase and the seminal contribution of Prof. Longa

Mikhail Osipov<sup>1,\*</sup>

The discovery of the twist-bend nematic phase (NTB) can be considered as one of the most significant recent achivements in the field of liquid crystals. In the NTB phase the director is tilted at constant angle  $\theta$  and forms a heliconical structure with nanoscale pitch which appears despite the achiral structure of the constituent molecules. From the general soft matter point of view the NTB phase can be considered as the first example of spontaneous chiral symmetry breaking in a fluid.

We discuss the existing Landau-de Gennes theory of the nematic twist-bend phase as well as the corresponding molecular models with the special emphasis on the contribution made by Lech Longa. In particular we consider the stabilization of the twist-bend structure, the role of the flexoelectric effect and the softening of the bend elastic constant, and the role of the local biaxial ordering.

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### Presentations (continued)

Wednesday 27/09, 12:10 - 12:50

## Topological constraints of activity-driven transitions from stationary defect dynamics to nematic turbulence

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Confined nematic liquid crystals are characterized by the interplay of ordering, elasticity, chirality, confinement, surface anchoring, external fields, flows, and activity that leads to numerous complex static and dynamic structures, including singular topological defects and nonsingular solitonic deformations. Increasing interest in active soft matter stimulated us to analyze topological aspects of three-dimensional extensile activity-driven nematodynamics topologically constrained by spherical confinement [1,2]. We used a simple mesoscopic modeling of active nematic fluids [3] that enables numerical simulations of active nematodynamics which reasonably well describes experiments with active complex fluids in thin layers and shells. These are mostly biological systems driven by the internal conversion of stored chemical energy into motion [3,4]. We demonstrated that at low activity stationary dynamic structures occur that with increasing activity undergo transitions from stationary to chaotic 3D motions - active nematic turbulence. In this seminar, I will present how the time evolution in a such system can be for a specific confinement characterized by a series of elementary topological events where nematic disclinations divide, merge, annihilate, and crossover. We limit our discussion to homeotropic anchoring, no-slip surface, and for selected activities illustrate our findings by simulated dynamics of nematic disclinations & flows accompanied by simulated optical microscopy. Our simple confined system could be a nice test ground for a machine-learning approach to active nematics [5].

The research was done in collaboration with S. Čopar, J. Aplinc, Ž. Kos, and M. Ravnik.

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### Presentations (continued)

Wednesday 27/09, 12:50 - 13:30

## Complex helical smectic phases made of achiral molecules



Ewa Górecka<sup>1,\*</sup>

Intensive research focused on chiral liquid crystals (LCs) has been driven by their unique ability to exhibit tunable physicochemical properties and structural complexity, which can rival sophisticated natural materials. I will provide insights into liquid crystalline phases composed of achiral molecules that demonstrate chiral structure and/or chiral morphology. The discussion will begin with an exploration of recent advancements in the discovery of new classes of chiral LCs, made possible by the application of resonant X-ray scattering. This technique is sensitive to molecular orientation modulations, enabling the acquisition of information that is often challenging to obtain using other methods. The liquid crystalline phases serve as excellent examples of systems with inherent chirality capable of propagating across structures of varying length scales. The study delves into helical assemblies and the intriguing phenomenon of mirror symmetry breaking, which occurs spontaneously in materials where chirality emerges from achiral molecules.

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## Presentations (continued)

Wednesday 27/09, 15:00 - 15:40

## Some open questions in the elasticity of nematic liquid crystals: insights from microscopic theory

Alberta Ferrarini<sup>1,\*</sup> and Davide Ravignas<sup>1</sup>

The elastic behaviour of nematic liquid crystals is commonly interpreted on the basis of the Oseen-Frank free energy [1,2], in which the cost for distortions from the uniform alignment is decomposed into contributions corresponding to three modes – splay, twist, and bend - built from the first-order derivatives of the position dependent director. Typical low molecular mass thermotropic systems exhibit comparable elastic properties, weakly dependent on their chemical structure, which is in agreement with the prediction of classical microscopic theories [3]. Yet, the same does not apply to polymeric liquid crystals, whose elastic properties are still incompletely understood [4]. Recently, various examples of unusual elasticity have been highlighted: these include spontaneous twisting of the director in achiral chromonic liquid crystals, as well as an exceptionally low cost for bend or splay deformations in mesogens with unconventional shapes, which has been related to the formation of novel nematic phases [5]. In this talk we will discuss how, introducing new elements in the macroscopic theory [6], we can explain the variety of experimental behaviours.

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### Presentations (continued)

Wednesday 27/09, 15:40 - 16:20

## Nematic ordering in active systems IT

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Active systems refer to collections of entities that consume energy and thereby move forward showing emergent collective dynamics. In the macroscopic world this could be fish schools or flocks of birds. In the microscopic world, which we address here, the entities often have the shape of rods like bacteria or are flexible filaments such as microtubules, which are biopolymers found within cells. For sufficiently large densities the active entities exhibit local orientational order and may even show active turbulence.

The talk addresses such systems from two perspectives. First, we use full hydrodynamic simulations of a collection of active rods moving in their fluid environment. We show the dynamic ordering, which arises as a function of density and the aspect ratio of the rods using different types of microswimmers, namely pusher, puller, or neutral active rods. In particular, pusher swimmers can exhibit turbulent motion.

In the second part, we rely on a continuum description of active paranematics, the Doi-Edwards theory supplemented by active stresses. Above an absolute pusher strength, activity induced nematic ordering arises, where disclinations continuously form or annihilate each other. We show how this active turbulence can be controlled by a lattice of inactivity spots leading to multi-lane flow and confined vortex states.

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### Presentations (continued)

Wednesday 27/09, 16:20 - 16:45

## A self-consistent mean field model for hard ellipsoids CT

<u>Peter Palffy-Muhoray</u><sup>1,2,\*</sup>, Epifanio Virga<sup>3</sup>, Jamie M. Taylor<sup>4</sup>, Thomas Fai<sup>5</sup> and Xiaoyu Zheng<sup>1</sup>

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Assemblies of hard ellipsoidal particles form orientationally ordered phases with increasing number density. A simple self-consistent mean field model is proposed to study the transition from the isotropic to the nematic phase. The simplicity of the model gives ready access to the order parameter, free energy and pressure, in good agreement with simulations. The model may be useful to describe photomechanical stresses in liquid crystal elastomers due to photoisomerization.

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## Presentations (continued)

Wednesday 27/09, 17:15 - 17:40

## Entropy-driven formation of modulated and frustrated mesophases in a system composed of bent-core molecules CT

Piotr Kubala<sup>1,\*</sup>, Wojciech Tomczyk<sup>1</sup> and Michał Cieśla<sup>1</sup>

Since their discovery, liquid crystals have found countless applications, with the most prominent being liquid-crystal displays (LCDs). The simplest liquid crystalline phase is a uniform nematic, where all molecules align along a constant preferred direction called the director. However, in some systems, the director acquires spontaneous spatial modulation. Examples of such phases include cholesteric, splay-bend nematic, splay nematic, and twist-bend nematic. There are also systems where the director and polarization fields are not continuous, i.e., spatial defects are present. Frustrated phases, such as  $B_1$  and  $B_7$ , have been experimentally observed for banana-shaped molecules. Many phenomena can be attributed to entropic forces. Several computational studies have shown that phases such as twist-bend nematic or splay-bend smectic can be found in hard-core systems of bent-core molecules. In this study, we focused on one of such models. We conducted Monte Carlo simulations of banana-shaped molecules composed of hard tangent spheres with a fixed bend angle and a variable number of spheres. The main goal was to assess the stability of modulated phases. Additionally, we observed a frustrated B<sub>1</sub> polar blue phase, which, to our best knowledge, had not been previously reported within a computational study. The talk emphasizes the geometric and entropic factors that lead to the self-assembly of the reported structures.

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## Presentations (continued)

Wednesday 27/09, 17:40 - 18:05

# Properly dealing with recent discoveries in suspensions of bent colloidal rods by means of a grand-canonical Landau-de Gennes theory CT

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Bent-core liquid crystals are mesophases formed by molecules having a "banana-like" shape that favors spontaneous bend deformations in the nematic director field. As a pure bend deformation cannot uniformly fill 3D space, Meyer and later independently Dozov argued that these local bend deformations should be accompanied by either a twist or a splay deformation [1]. In the former case, they theoretically postulated the stabilization of a spatially modulated twist-bend nematic  $(N_{\rm SB})$  phase; in the latter case, they predicted the onset of a spatially modulated splay-bend nematic  $(N_{\rm SB})$  phase.

While most of the research on bent-core liquid crystals has focused on thermotropic bent-core mesogens that become liquid crystalline upon lowering the temperature, very recently various routes have been developed to synthesize lyotropic colloidal model systems of bent particles whose liquid crystalline behavior is driven by concentration.

In this context, a stable  $N_{\rm SB}$  phase has been experimentally observed (for the first time!) in a system of smoothly curved colloidal rods [2] and later in polydisperse bent silica rods [3]. However, the nematic nature of the discovered phases has been questioned. Recent simulations [4], indeed, have showed the (alleged)  $N_{\rm SB}$  phases to display density modulations, which cannot be described by current Oseen-Frank and Landau-de Gennes type theories [1].

Using a novel grand-canonical Landau-de Gennes theory for colloidal suspensions of bent rods [5], we investigate [6] how spatial deformations in the nematic director field affect the local density of  $N_{\rm TB}$  and  $N_{\rm SB}$  nematic phases. The grand-canonical character of our theory naturally relates the local density  $\rho$  to the local nematic order parameter S. In the  $N_{\rm SB}$  phase, we find S and hence  $\rho$  to modulate periodically along one spatial direction. As a consequence the  $N_{\rm SB}$  phase has the key symmetries of a smectic rather than a nematic phase. By contrast, we find that S and hence  $\rho$  do not vary in space in the  $N_{\rm TB}$  phase, which is therefore a proper nematic phase. We argue the density modulations to be inherently coupled to splay deformations in the nematic director field.

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## Presentations (continued)

Finally, we employ our theory to study the first-order  $N-N_{\rm TB}$  phase transition observed in simulations of hard bent spherocylinders [4]. We find that the bend elastic constant  $K_{33}$  as well as its renormalized version  $K_{33}^{\rm eff}$  remain positive at the transition, whereas  $K_{33}^{\rm eff}$  vanishes at the nematic spinodal. This finding appears to be general and could help in understanding the problem of the softening of the elastic constants in systems with spontaneous polar order.

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### Presentations (continued)

Thursday 28/09, 09:00 - 09:25

### Mitosis of life aims in Poland 2012-2016 CT

Maciej Wołoszyn<sup>1</sup>, Maria Nawojczyk<sup>2</sup>, Maria Stojkow<sup>2</sup>, Dorota Żuchowska-Skiba<sup>2</sup>, Grzegorz Ptaszek<sup>2</sup> and Krzysztof Kułakowski<sup>1,\*</sup>

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From European Social Survey 2012-2016, data are selected on how Polish respondents are attached to 21 issues. The list of issues is formulated according to the scheme: 'it is important to ...' and it includes items like: try new and different things, make own decisions, seek fun, follow traditions, behave properly etc. The answers are weighted according to 6-point Likert scale. The Pearson correlation coefficients r(i,j) are calculated between the profiles of attachment to particular issues i,j as dependent on education of the respondents. Further, the coefficients r(i,j) are used as initial values of the relations s(i,j) between the issues, governed by the differential equations ([1] and literature therein)  $\frac{ds(i,j)}{dt} = [1-s^2(i,j)] \sum_k s(i,k)s(k,j)$ .

Generically, the solutions s(i,j) tend to  $\pm 1$  in such a way that two separate groups of issues arise, with s(i,j)=+1 for i,j within the same group and s(i,j)=-1 for i,j in distinct groups. In this way we refer to the concept of Heider balance, applied here to the issues which represent life aims; hence the term 'mitosis' in the title.

There is a clear continuity of the results, repeated through three rounds in 2012, 2014 and 2016. Namely, the partition changes for only 4 out of 21 issues. We are going to discuss to what extent the content of each group is coherent. In this set of items we could distinguish coherent two sets of attitudes. One – say, group A - is representative of achieving society as David McClelland described it in his famous book [2]. These are proactive driven by different motivations, creative, open minded people. Second – group B - are people with 'traditional' attitudes of being modest, obedient, follow rules, rather be subordinated that being a leader – traditional conservatives. There are few labile items, we will follow their inclusion or exclusion to define groups describing the broader context in which they occurred.

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### Presentations (continued)

Thursday 28/09, 09:25 - 09:50

## Reentrant phase transition in the TASEP with parking spots

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Understanding vehicular dynamics in urban areas is a central task for modifying urban space planning and implementing effective policies to optimize transportation time and reduce carbon dioxide emissions. Incorporating parking slots is crucial as parking maneuvers and cruising for parking impact vehicular flow. From a microscopic perspective, vehicular traffic can be treated as interacting particles driven far from equilibrium. One of the simplest out-of-equilibrium models is the Total Asymmetric Exclusion Process (TASEP), which has been analytically solved with open boundaries.

To focus specifically on urban traffic, we propose a TASEP variant that includes a parking spot at each site, occupied by at most one particle. Two types of particles have been considered: slow particles that attempt to park at a given rate if a parking spot is available, and fast particles that cannot park. Parked particles return to the road as fast particles at a specified rate, if feasible. This general model encompasses several previously studied TASEP variants. Dynamical properties and phase diagram have been investigated using Kinetic Monte Carlo simulations, exact diagonalization of the stochastic matrix, and mean field theory.

We have shown the non-monotonic behavior of the current with respect to the input rate and parking rate, leading to re-entrant phase transitions. This novel behavior remains robust when introducing disorder in the parking and leaving rates, as well as when employing a different update scheme, namely the parallel update. Shifting the parking area within the bulk reveals properties similar to TASEP with a finite-size bottleneck which can be controlled through the parking and leaving rates.

These non-trivial dynamics underscore the importance of carefully choosing these rates and the placement of parking spots to maximize vehicular flow.

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### Presentations (continued)

Thursday 28/09, 09:50 - 10:15

## Nonconservative diffusion processes CT

Piotr Garbaczewski<sup>1,\*</sup> and Mariusz Żaba<sup>1</sup>

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We analyze pros and cons of the recently introduced theoretical framework, within which the dynamics of nonequilibrium diffusion processes is related to the fully Euclidean version of the Schrödinger quantum mechanics with a minimal electromagnetic coupling. The arising "magnetic"affinity is set against the standard theory of the Brownian motion in a magnetic field. The benefit is that the existing exact formulas for transition probability density functions of the involved Markovian diffusion processes, can be mapped into their (merely formal) path integral counterparts in the non-Hermitean setting of [Phys. Rev. E 107, 014101, (2023)]. This allows to discriminate beween the standard Brownian magnetic lore and potentially useful electromagnetic analogies appearing in the study of nonconservative diffusion processes, which do not necessarily embody the very concept of electromagnetic perturbations of diffusing charged particles, but extend far beyond this setting.

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### Presentations (continued)

Thursday 28/09, 10:45 - 11:25

## Random walks in correlated diffusivity landscapes IT

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Diffusion of particles in random, correlated diffusivity landscapes can serve as one of the models leading to the so-called Brownian yet non-Gaussian diffusion. Under the corresponding choice of parameters, the model leads to the mean squared displacement of particles growing linearly in time, with the probability density function (PDF) of displacements changing its shape from a double-sided exponential (Laplace) at short times to a Gaussian at long ones [1]. The art of convergence to a Gaussian is, however, unusual: under the rescaling implied by the Central Limit Theorem, the central peak of the initially two-sided exponential PDF doesn't smoothen and lower but stays high while getting narrower [2]. This kind of behavior is not reproduced by the mean field theories of the phenomenon like continuous time random walks (CTRW) or diffusing diffusivity models. We discuss this kind of unusual behavior, and show that it is caused by strong correlations between spatial and temporal aspects of the motion, and cannot be reproduced by correlated CTRW schemes neglecting spatiotemporal correlations even if full temporal memory is included. Therefore, observation of the persistent central peak in the PDF could indeed serve as a clear hint onto strong, correlated spatial disorder in the system.

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### Presentations (continued)

Thursday 28/09, 11:25 - 11:50

## Statistical properties of random advection-diffusion CT

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We study the statistics of a one-dimensional randomly advected field with diffusion. The motivation for this setup comes from a straightforward interpretation as advection of particles in one-dimensional turbulence, but it is also related to a problem of synchronization of dynamical systems driven by common noise. A general class of lattice models describing the joint effect of random advection and diffusion for an ensemble of particles is introduced. It consists of a general microscopic random update rule and encompasses as specific cases, some models studied in the literature, like the Kang-Redner, Kipnis-Marchioro-Presutti, Takatasu-Taguchi etc. For finite lattices, we study both the coagulation of an initially spread field (interpreted as roughening), and the statistical steady-state properties. We distinguish two main size-dependent regimes, depending on the strength of the advection term and on the lattice size. Using numerical simulations and mean-field approach, we study the statistics of the field. For weak diffusion, we unveil a characteristic hierarchical structure of the field. We also connect the model and the iterated function systems concept.

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## Presentations (continued)

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## Dynamical phase transition in the fluctuations of occupation fraction of N non-crossing Brownian particles $\Box$

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The study of the dynamics of occupation time has a variety of applications. For example, it has been used to analyze the morphological dynamics of interfaces, analysis of the fluorescence intermittency emitting from colloidal semiconductor dots, optical imaging etc to name a few. The occupation time dynamics have been studied for numerous problems in the context of non-equilibrium systems. In this work we study the large deviation statistics of occupation fraction of N non-crossing Brownian particles in a certain interval. Using the extension of the Donsker-Varadhan formalism we solve this problem by mapping it to N non-interacting spinless fermions trapped in a square well potential. We study the behaviour of the large deviation function for all  $N \geqslant 1$ . For N=1, the single Brownian motion in presence of a drift is known to exhibit dynamical phase transition of first order where the large deviation function shows singularity. For any  $N \geqslant 2$ , we interestingly find that the system undergoes multiple dynamical phase transitions of second order. This phenomenon is entirely different from what is found for a single Brownian motion occupation fraction. Here each transition denotes different numbers of particle occupations near the vicinity of the interval.

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### **Posters**



## How to use liquid state theory to predict jamming of hard spheres

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Slow compression of a hard-sphere fuid at constant temperature yields an entropy-driven first-order transition from the liquid to a crystalline phase [1,2]. When the fuid is compressed quickly rather than slowly, however, crystallization can be avoided and the particles "jam" in a disordered configuration. The determination of the so-called *random close packing* (RCP) density, defined as the highest packing fraction for a disordered arrangement of hard spheres, remains an open problem [3].

In a recent paper [4], it was attempted to use liquid-state theories to analytically determine the RCP density of a monodisperse hard-sphere fluid. After combining a well-defined criterion for the onset of shear rigidity at jamming with a direct quantitative link between the contact value of the radial distribution function g(r) and the kissing number z; existing equations of state for hard spheres were shown to be succesfull in predicting the RCP density either in d=2 and d=3 dimensions.

Here [5], we back up the analytical scheme introduced in [4]. We show that, when the notion of maximally random jammed (MRJ) state [3,6] is generalized to that of MRJ-line, the Percus-Yevick and Carnahan-Starling equations of state capture the density dependence of z for a family of numerically generated jammed states of hard spheres. Consequently, it is reasonable to assume the most random branch of jammed states to undergo crowding in a way qualitatively similar to an equilibrium liquid. We prove that, for hard-sphere systems, liquid-state theories can be successfully used to estimate RCP, when the latter is identified with the densest isostatic point, i. e. the densest among the MRJ states with z=6.

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### Posters (continued)

Our finding is further enforced by the analysis of polydisperse systems. Either in the case of bidisperse and polydisperse hard spheres our prediction of RCP is in very good agreement with simulations, for a large values of size ratios and polydispersity. Finally, a perturbative expansion yields a closed-form expression for RCP that quantitatively captures a distribution-independent regime for small size polydispersities.

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## Posters (continued)



## Microscopic theory for the shear-induced structure distortion in concentrated suspensions of spherical colloids

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A major challenge in soft matter physics is to understand the repercussions of an external shear flow on the microscopic structure of colloidal suspensions. In the case of diluted suspensions of spherical colloids, a common starting point for the theoretical treatment of the problem is the two-body Smoluchowski *convection-diffusion* equation [1]. However, solving the latter equation is typically challenging even numerically, due to the *boundary-layer* behaviour shown at large separations among the colloidal particles [2].

An approximate analytical solution to the Smoluchowski convection-diffusion equation fully taking into account the boundary-layer structure, was recently found by means of matched asymptotic expansions [3]. We here show that combining this analytical solution with generalized integral equations of the liquid state, allows us to investigate the shear-induced structural distortion in concentrated regimes of packing fraction  $\eta$ ; so far explored only by means of numerical simulations.

We consider both the case of hard spheres [4] and that of hard-core repulsive Yukawa particles [5], under shear flow. We compute the pair correlation function and extract scaling laws for its contact value. For hard spheres, our findings are in very good parameter-free agreement with numerical data from literature [6], up to  $\eta \approx 0.5$ . In addition, our scheme predicts (for the first time) a consistent enhancement of the structure factor S(k) at  $k \to 0$ ; upon increasing the shear rate, which we argue may signal the onset of a shear-induced phase transition from the isotropic phase to a non-uniform one.

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## Posters (continued)

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### Posters (continued)



## Subdiffusion in a randomly inhomogeneous medium from a Fock space approach

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In this work we study the problem of a random walk in a finite-size randomly inhomogeneous one-dimensional medium by using a Fock space approach. We map the master equation of the walker into a Schrödinger-like equation and we describe the evolution of the random walk in a Fock space in which the system states are assigned to the sites of a regular one-dimensional lattice. This formalism allows to evaluate the probability P(i,t) of finding the walker in a given point i at a given time t. Unlike previous applications of a Fock space for random walks displaying anomalous diffusion [1,2], here we set in each point i of the domain the probability  $r_i \in [0,1]$  for the walker to stay and the symmetric probabilities  $(1-r_i)/2$  to jump on the left or on the right, respectively, into the nearest neighbor site. Moreover, probabilities  $r_i$  are assumed to be random and drawn from a Beta distribution B(a,b) in each i-site of the domain. If b < 1, then a crossover from standard to sub-diffusion is observed. We show that the walker distribution converges to a stretched-exponential in the case of subdiffusion and the functional relation between the anomalous exponent and the statistical features of  $r_i$  distributed according to B(a,b) is also provided.

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### Posters (continued)



## Giant enhancement of transport induced by active fluctuations via periodic potential

Karol Białas<sup>1,\*</sup> and Jakub Spiechowicz<sup>1</sup>

Understanding the role of active fluctuations in physics is a problem emerging both as a hot topic and a major challenge. The reason for this is their inherent non-equilibrium nature. This feature opens a landscape of phenomena yet to be explored that are absent in the presence of thermal fluctuations alone. Recently a paradoxical effect has been briefly communicated in which a free particle transport induced by active fluctuations in the form of white Poisson shot noise can be enormously boosted when it is additionally subjected to a periodic potential by exploiting relaxation down the potential slope. Here, the original predictions are considerably extended, and the impact of statistics of active fluctuations on the occurrence of this effect is investigated. A toy model of the jump-relaxation process is constructed, which allows for the identification of different transport boost regimes and explanation of their corresponding mechanisms and consequently pinpointing properties of active fluctuations statistics necessary for the effect to occur. The results are relevant not only for microscopic physical systems but also for biological ones such as e.g., living cells where fluctuations generated by metabolic activities are active by default.

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### Posters (continued)



### A stochastic model of translocation of knotted proteins

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Knotted proteins can become jammed when forced through pores if the knots in their back-bone tighten under force. Alternatively, the knot can slide off the chain, enabling translocation. This process can be described using a simple energy landscape model with a time-periodic potential that mimics the action of a molecular motor. Such a stochastic model exhibits similar behaviour to results obtained from molecular dynamics but has the advantage of simplicity and interpretability with only a few parameters. This talk will present the model along with results for translocation time as a function of the period of the pulling force and discuss the asymptotic limits and biological relevance of the findings.

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### Posters (continued)



## Numerical simulation of Lévy flights diffusion with drift in heterogeneous membranes

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Understanding transport processes through membranes require the modeling of diffusion, particularly when it comes to enhancing process effectiveness. The goal of this research is to understand the relationship between membrane structures, external forces, and the characteristic features of diffusive transport. We investigate Cauchy flight diffusion with drift in heterogeneous membrane-like structures. The study focuses on the numerical simulation of particle movement across different membrane structures with differently spaced obstacles. Four studied structures are similar to those of sodium alginate membranes filled with iron oxide nanoparticles. The other three structures were designed specially to show the crucial factors that affect most diffusional transport under the influence of drift. The movement of particles driven by Cauchy flights is compared to a Gaussian random walk both with and without additional drift action. We show that effective diffusion in membranes with an external drift depends on the type of internal mechanism that causes the movement of particles as well as on the properties of the environment. In cases of weak drift, the effective diffusion is fully determined by the environment (i.e., the properties of the membranes), whereas the internal mechanism (i.e., Cauchy flight or Brownian motion) does not matter. Superdiffusion is typically observed when movement steps are provided by the long-tailed Cauchy distribution and the drift is sufficiently strong. On the other hand, strong drift can effectively stop Gaussian diffusion.

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## Non-equilibrium fermionic transport in a periodically-driven tilted lattice

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Investigation of non-equilibrium fermionic transport in a periodically-driven tilted lattice is currently a subject of major interest. Transport properties in this setting are influenced by the drive, tilt, and interactions, as well as the non-Markovian nature of the fermionic reservoirs. We address this setup with two complementary tools, with an ultimate aim at addressing the interplay of all four of these factors in transport: We first formulate quantum transport of driven systems within the extended reservoir approach (ERA), which provides a method to capture continuum reservoirs with both a finite bandwidth and a finite bias. As with non-equilibrium steady states in time-independent scenarios, the current displays a Kramers' turnover including the formation of a plateau region that captures the physical, continuum limit response. We demonstrate that a simple stability criteria identifies an appropriate relaxation rate to target this physical plateau. To benchmark this criteria, we study a non-interacting, one-dimensional driven tilted lattice. The approach recovers well-understood physical behavior in the limit of weak system-reservoir coupling. Extended reservoirs enable addressing strong coupling and nonlinear response as well, where we analyze how transport responds to the dynamics inside the driven lattice. In second step, we introduce a many-body density-density interaction and study transport in the fully Markovian limit (e.g., infinite bandwidth and bias). At weak many-body interaction (and weak system-reservoir coupling) the rotating wave approximation captures the various resonance that appear due to the periodic drive. As the many-body interaction increases, a new resonance appears that can display a giant enhancement of conductance. The next step is to put these two sets of results together within tensor networks and study fully many-body quantum transport in a periodically driven system in the presence of finite bias, finite bandwidth reservoirs.

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### Posters (continued)



## Necessity for coarse graining empirical densities and currents in continuous space

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We present general results on fluctuations and spatial correlations of the coarse-grained empirical density and current of diffusion on all time scales in equilibrium or non-equilibrium steady states [1,2] and for transient or non-ergodic dynamics [3]. The time averaging and coarse graining hardwired in the definition of the functionals under consideration give rise to experimentally relevant but highly non-trivial statistics. We unravel a deep connection between current fluctuations and generalized time-reversal symmetry. We highlight the essential role of coarse graining in space from mathematical, thermodynamical, and experimental points of view. Spatial coarse graining is required to uncover salient features of currents that break detailed balance, and a thermodynamically "optimal" coarse graining ensures the most precise inference of dissipation. The results and employed methods give a new view on the Thermodynamic Uncertainty Relation [4]. Defined without coarse graining, the fluctuations of empirical density and current are proven to diverge on all time scales in dimensions higher than one, which has far-reaching consequences for large-deviation limits in continuous space. Our findings provide new intuition about time-averaged observables and allow for a more efficient analysis of single-molecule experiments.

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### Marginal fluctuation relations for currents

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The effective dynamics of stochastic systems with a finite number of states where only a few degrees of freedom are accessible to observation is described in terms of coarse-grained models. Coarse graining on states typically entails non-markovianity that is recovered under physically motivated assumption, thus restricting the range of applicability of such models. We use a novel approach based on occurrences of transitions to construct a coarse-grained description which provide the statistics of marginal currents up to the occurrence of a fixed number of transitions. In particular, a fluctuation relation for single currents is derived, and we extend its validity to an arbitrary number of observed transitions.

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## Quantifying active nematic turbulence

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Biological systems ranging from cytoskeletal networks to bacterial suspensions and epithe-lial monolayers exhibit complex chaotic flows known as active turbulence. Countless active molecular interactions combine to form a turbulent mix of behaviours, with fascinating non-equilibrium properties. With an eye to developing a quantitative understanding, we study turbulence and spatiotemporal chaos in 2D active nematics. Combining theory and GPU-accelerated simulations, we quantify characteristics of this activity-dependent chaos using correlations, non-Gaussianity of distributions, and finite-time Lyapunov exponents and their associated vectors. These numerical results are compared with data from microtubule-kinesin active nematics experiments. These analyses allow us to place active turbulence within the framework of dynamical systems, providing a more holistic, quantitative understanding of this phenomenon.

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#### Posters (continued)



## Velocity-fluctuation-induced anomalous kinetics in multispecies reaction-diffusion system

Matej Kecer<sup>1,\*</sup>, Michal Hnatič<sup>1,2</sup> and Tomáš Lučivjanský<sup>1</sup>

We investigate the anomalous kinetics of two-species reaction-diffusion system  $A+A\to (\emptyset,A),\ A+B\to A$  near its upper critical dimension  $d_c=2$ . In particular, we analyze an advection of reactants by random velocity field generated by the stochastically forced Navier-Stokes equation. The model is analysed by means of field-theoretic renormalization group (RG) and two-parameter  $(\epsilon,\Delta)$  expansion. Here  $\epsilon$  denotes deviation from Kolmogorov scaling and  $\Delta$  is deviation from space dimension d=2. The RG analysis is performed to leading order in perturbation scheme and all stable macroscopic regimes are identified.

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## Modeling tumor growth with the Allee effect

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To describe the growth of a cell colony, processes such as cell division, cell death and cell movement must be taken into account. All of these mechanisms can have multiple contributing factors, and one of them is the density of cells in the surroundings. It is often assumed that the growth of cancer cell colonies is characterized by an exponential increase in the number of cells, and a decrease in the rate of colony growth is only considered in large populations when cells have limited access to resources such as nutrients, oxygen or space. However, studies indicate that in small populations of cancer cells the Allee effect can be observed [1]. The allee effect is a phenomenon that is characterized by the per-capita growth rate of a population being low or even negative at small population sizes. To describe tumor growth at the initial stages, a stochastic model was proposed, that took into account the effect of local cell density on cell division. The model results in slower growth in the initial stages of colony development, as described in the literature.

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#### Posters (continued)



## The role of tissue in micro indentation tests of a plant cell

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Classical measuring methods used in material engineering are not suited for biological tissues, especially in microscale. It is almost impossible to produce a homogenous specimen of biological material for a classical tensile test. Indentation experiments are much easier to perform on a microscopic object like a cell. However, this comes at a cost: interpretation of the results. Extracting material properties from an indentation experiment is a serious issue, and it becomes more difficult for inhomogeneous "materials", for example cells. And for a system as complex as tissue, there is no other method for extracting material properties than the one utilizing finite element simulations. In these simulations, it is crucial to know in what range the indentation experiment affects the tissue to optimize simulations.

Plant tissue works mechanically like an inflatable mattress. The rigidity comes from pressure exerted on the internal side of cell walls. The pressure of the cytoplasm is crucial to the tissue's mechanical behavior. There are two approaches to modeling the pressure. One is to exert constant pressure on the inner side and the other is to treat cytoplasm as incompressible liquid. The difference between the two models is exceptionally pronounced in the case of the 2D tissue-like epidermis. Here we present the results of the indentation of a 2D tissue of several sizes starting from a single cell. Comparison between the following models: constant pressure and hydrostatic, helps to understand how the force induced by indentation propagates along the tissue. This assessment of the maximal distance probed by the indentation experiment will help in the long-term goals of measuring the properties of the cells in tissue.

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#### Posters (continued)



## Mapping the space of Turing patterns

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Patterns arise in nature at different scales. We can recognize animals based on their furry patterns alone, from the spots on a leopard to the stains on a cow. However, patterns are established also during embryonic development, through interactions of diffusing molecules that activate expression of target genes. As a result a striped pattern of gene expression emerges. These stripes will later on give raise to different body parts and organs. What is amazing is that this pattern is established with precision of a few cell diameters, being robust against perturbations from a noisy cellular environment. How this level of patterning reproducibility and robustness is achieved for each new organism is the central question of developmental biology.

We address this question by using concepts developed by Alan Turing. We focus on studying patterns emerging in systems with reaction-diffusion equations describing spreading and interactions of different chemical species (morphogens) inside the embryo. By analytically calculating conditions for parameters that need to be satisfied to observe diffusion driven instabilities that result in a spectrum of stable spatial patterns we define the Turing space. In this Turing space we investigate robustness of patterns against perturbation in parameters by identifying size and shape of regions resulting in the same number of stripes. We investigate systems with two and three interacting morphogens.

First, we show that for systems of infinite size their Turing space becomes a projective space. Thanks to scale invariance and other symmetries, we are able to find basis vectors whose linear combination parametrize the whole Turing space. This allowed us to derive explicit formulas for the robustness of patterns. Second, we use the properties of Turing space of infinite size systems to study the Turing space for finite size systems. We proved that Turing space is still connected, infinite and certain boundaries are also scale invariant. Similarly, we derived bounds and approximations for the robustness of patterns. Taken together, our results provide tools for both faster numerical exploration of Turing space, as well as for testing whether regions of Turing space indicating the highest robustness of patterns correspond to patterns observed in actual biological systems.

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#### Posters (continued)



## **Emergent order in single-file active Ornstein-Uhlenbeck particles conditioned on dissipation**

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Active work quantifies the amount of energy converted into the actual motion of active particles. In the long-time limit, the time-averaged active work quantifies how much energy is dissipated by active particles into the surrounding environment, i.e., it is a measure of the entropy production rate of active particles. Thus, by calculating the large deviation function (LDF) of the time-averaged active work in the long-time limit, we can gain information about (i) the likelihood of an atypical energy dissipation rate and (ii) what the system looks like when such atypical events occur. A previous study on two-dimensional active Brownian particles [1] showed that the LDF exhibits singularities associated with transitions from the collectively moving state via the phase-separated state to the phase-separated arrest state, in the order of decreasing entropy production rate. In our study, we focus on the case of one-dimensional active Ornstein-Uhlenbeck particles, which corresponds to the active particles moving in a single-file along a narrow one-dimensional channel. In contrast to the previous study, we find in this case that the collective motion can be induced by decreasing the entropy production rate, and that further decrease of the entropy production rate induces another transition to a crystal state, where active particles effectively repel each other. Our results are based on a recently proposed machine learning method that utilizes the stochastic optimal control theory [2].

#### References

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## Posters (continued)



## Thermodynamically consistent modeling of fuel-driven active engines: effects of the self-propulsion parity

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Engines powered by active particles are well-known for their exceptionally high performance: their efficiency can surpass the Carnot efficiency while simultaneously achieving positive power. However, this 'super-Carnot' behavior arises from considering the apparent statistical signature of the system as a whole, without distinguishing heat and work.

Consequently, this 'apparent' description of active heat engines cannot explain how their performances are eventually limited by thermodynamics. To address this issues, thermodynamically consistent theories of active heat engines should be developed.

In this paper, we first develop a theoretical framework which enforces the (anti-)symmetric structure of coupling coefficients between variables so that the system is guaranteed to reach thermodynamic equilibrium in the absence of external driving. Next, we consider a mechanochemical coupling between a colloidal particle's positional coordinate and a constant chemical driving. This maintains the particle far from equilibrium, resembling the dynamics of the AOUP which is a renowned model of active particle. Additionally, the dynamics of fuel consumption is decided based on the constrained structure of coupling.

Meanwhile, a controversy regarding the thermodynamics of active matter is the behavior of the self-propulsion forces under time reversal. Some literature assume that the sign of self-propulsion force remains unchanged under time-reversal (even-parity), while others assume it changes (odd-parity). Depending on these parity interpretations, two distinct formulas of 'active work' (the energy supplied to the particle) are reported.

Using our general framework, we first show that both formulas can be nontrivially recovered under the assumption of tight mechanochemical coupling. This top-down argument demonstrates that that both formulas are possible depending on the specific mechanism of self-propulsion. In addition, we report that the Clausius relation precisely holds between the heat dissipation of the AOUP identified from the first law of thermodynamics, and the entropy production (EP) defined from the path probabilities using the standard tool of stochastic thermodynamics.

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#### Posters (continued)

Next, we construct an active heat engine with this chemically driven AOUP. From the Clausius relation above, we define a novel concept of efficiency for this engine, which contains both heat injection and chemical fuel consumption in the denominator. This new efficiency is properly bounded from above by the second law of thermodynamics. Also, we can recover the previously reported 'apparent' efficiency, providing a clear energetic picture for its super-Carnot behavior.

Another major advantage of this efficiency is that we can address the self-propulsion parity. The efficiency at maximum power (EMP) exhibits a surprisingly simple criterion: the even-parity (odd-parity) engine's EMP is better when the size of the engine is smaller (larger) than the persistence length of the active particle. Also, the EMP depends nonmonotonically on the strength of chemical driving, allowing the EMP of active case being larger than the passive case although the large fuel consumption is properly considered. We finally discuss the existence of a tighter upper bound on the efficiency of the odd-parity engines stemming from the detailed structure of the EP.

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## Posters (continued)



# Unveiling the connection between the critical exponents and the fractal dimension at a phase transition

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We develop the hypothesis that the dynamics of a given system may lead to a fractal dimension df different from the original spatial dimension d. This phenomenon is more easy to observe near a phase transition. We also speculate how the response function might be sensitive to this change in dimensionality. We discuss how this phenomenon appears in phase transition and growth phenomena [1-5]. We determine exactly the fractal dimension  $d_f$  for the Ising model and validate it via computer simulations for two dimensions.

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#### Posters (continued)



# Instabilities in helical magnetohydrodynamic turbulence: two-loop approach

Andrei Ovsiannikov<sup>1,\*</sup>

Magnetohydrodynamic (MHD) turbulence driven by the stochastic Navier-Stokes equation always has been a subject of intense study. In an electrically conducting media developed turbulence has a number of specific properties associated with magnetic field fluctuations which under certain conditions can increase and lead to the formation of a non-zero average large-scale magnetic field. This effect is known as a turbulent dynamo and is associated with the conservation of magnetic helicity. It is especially pronounced in systems with violated parity. Our research uses field-theoretic methods to propose a general scenario for the generation of arising homogeneous magnetic fields due to the mechanism of spontaneous symmetry breaking. We perform high-order calculations of self-energy Feynman diagrams responsible for the generation of a homogeneous magnetic field and its renormalization. In order to refine earlier one-loop results for the value of spontaneous magnetic field and deformation of Alfven waves in this model, we employ two-loop calculations. The investigation herewith focuses on studying the system's stability, which is necessary for the self-consistency of previously made predictions about the mechanism of system stabilization.

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#### Posters (continued)



# Numerical search for dipolar liquid phase in Abelian gauge quantum Hamiltonians

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Recent developments in experimental condensed matter physics allow for realization of Abelian gauge Hamiltonians on routinely controllable systems (Josephson junction arrays, optical lattices, etc). This opened the prospect of simulation of the phenomena of compact quantum electrodynamics and quantum chromodynamics (e.g, quark confinement) in the laboratory setup.

We consider  $Z_N$  symmetric generalized Bose-Hubbard Hamiltonian on a two-dimensional lattice. However, field theory predicts that it exhibits the confined phase, the gapped phase, one-dimensional Bose liquid phase, or gapless dipolar liquid phase. The latter two are particularly interesting in view of AdS/CFT correspondence (and the latter one is believed to exist only at large N and small coupling g). Our goal is search for these two phases (gapless dipolar liquid is most intriguing) by numerical methods.

The Hamiltonian is re-written in the second order of the perturbation theory and transformed so that it acts on a dual cylinder lattice. Its ground state is approximated by matrix product state (MPS) and evaluated using infinite-size density-matrix renormalization group (iDMRG). We calculate the von Neumann entanglement entropy as function of g for each N. The discontinuities of its first derivative signal the phase transitions, and the type of these transitions (or entire phases) is identified by the central charge:  $S = (c/6) \log \zeta + S_0$ .

Our calculations for N=2 indicate only one Ising-type phase transition with central charge c=1/2, and the system is in a gapped phase at large g. On the contrary, at N>2 the ground state of the system is highly degenerate at large g, and we have found no evidence of two phase transitions for N<6. The calculations for N=6 or larger are underway.

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#### Posters (continued)



#### Obstacle facilitated control of active nematics

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Active nematics are active fluids composed of elongated constituents in which force dipoles at the micro scale generate macroscopic flows. As in other active systems, bulk active nematics exhibit chaotic flows known as active turbulence. Unique to active nematics, however, is the existence of local orienational order, allowing the prescription of topological defects from various boundary geometries. In this work, motivated by recent experiments, we numerically model an active nematic in the presence of an array of obstacles of various shape and size. We show that the shape of obstacle induces defects of particular topology and that defects may be pinned by the obstacles. We use this, and the fact that positive defects are motile in active nematics, to realize control over the defect trajectories and flows in the system. We demonstrate various dynamical phases that depend on the strength of active force and geometry of the obstacles.

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## Posters (continued)



## Combination of two types of disorder in lattice random walk

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Often the motion in complex systems is subdiffusive. Meaning, instead of a linear dependence on time, the mean square displacement (MSD) grows as  $\sim t^\alpha$  where  $0<\alpha<1$ . This can be attributed to long waiting times that cause a significant slowdown from the classical description of Brownian motion. But a slow down of the MSD can also arise from repeated collisions with obstacles in the media causing persistent memory and correlations in the system. For the first time the moments of displacement are found in a system with a quenched disorder of obstacles combined with a heavy tailed distribution  $(\sim \tau^{-1-\alpha})$  of waiting times causing subdiffusion. Our mathematical description consists of a biased tracer particle being pulled by an external force, hopping on a two-dimensional lattice where a fraction of the sites are inaccessible and act as a reflective obstacle. We present a new method to find the moments of the system in discrete time, i.e amount of steps N, and use subordination to include the heavy tailed waiting times and transition to continuous time. Correlations in time where the temporal disorder is quenched is also studied. Our analytical results fit perfectly to numerical simulations in the limit of low obstacle density and arbitrarily strong driving force.

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## A deeper look into many-body localized phases: Ergodic bubbles and correlation function differences

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We present two approaches to explore the dynamics of many-body localization (MBL) in disordered interacting quantum systems using experimentally measurable single- and two-site correlation functions.

First [1], we propose an algorithm based on neural networks that uses two-site correlation functions to detect ergodic bubbles, i.e., delocalized regions surrounded by a localized phase, with a spatial and temporal resolution. In the MBL regime, we observe that ergodic bubbles grow in size logarithmically with time and their size distribution follows an exponential decay. In the ergodic phase, the bubble size distribution is a power law. This supports the scenario of delocalization through an avalanche mechanism, providing insights into the thermalization mechanisms of disordered many-body systems.

Second [2], we introduce a correlation function difference (CFD) based on local density correlations in a one-dimensional spin system. By studying CFD in ergodic, Anderson, and MBL regimes of a disordered XXZ spin chain, we analyze the dynamics of information transfer. In the ergodic phase, CFD propagates faster than spin transport but slower than the limit dictated by the Lieb-Robinson bound. In localized cases, we observe exponentially slow relaxation of CFD. The connections between CFD and other observables detecting non-local correlations are discussed.

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#### Posters (continued)



# Paradoxical nature of negative mobility in the weak dissipation regime

Mateusz Wiśniewski<sup>1,\*</sup> and Jakub Spiechowicz<sup>1</sup>

We reinvestigate a paradigmatic model of nonequilibrium statistical physics consisting of an inertial Brownian particle in a symmetric periodic potential subjected to both a time-periodic force and a static bias. In doing so we focus on the negative mobility phenomenon in which the average velocity of the particle is opposite to the constant force acting on it. Surprisingly, we find that in the weak dissipation regime, thermal fluctuations induce negative mobility much more frequently than it happens if the dissipation is stronger. In particular, for the very first time, we report a parameter set in which thermal noise causes this effect in the nonlinear response regime. Moreover, we show that the coexistence of deterministic negative mobility and chaos is routinely encountered when approaching the overdamped limit in which chaos does not emerge rather than near the Hamiltonian regime of which chaos is one of the hallmarks. On the other hand, at non-zero temperatures, the negative mobility in the weak dissipation regime is typically affected by the weak ergodicity breaking. Our findings can be corroborated experimentally in a multitude of physical realizations including e.g. Josephson junctions and cold atoms dwelling in optical lattices.

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#### Posters (continued)



# Growth kinetics of random sequential adsorption packings built of two-dimensional shapes with discrete orientations

Wiktor Zantowicz<sup>1,\*</sup>, Piotr Kubala<sup>1</sup> and Michał Cieśla<sup>1</sup>

We studied random sequential adsorption packings constructed from rectangles, ellipses, and discorectangles, where the orientations of constituent shapes were picked from discrete sets of values with varying spacing. It allowed us to monitor the transition between the two edge cases: the parallel alignment and the arbitrary, continuous orientation of the shapes within the packing. The packings were generated numerically. Apart from determining the kinetics of packing growth in low- and high-density regimes, we analyzed the results in terms of packing density and probed the microstructural properties using the density autocorrelation function.

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Notes	

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Notes	

	15:	15::	16:0	16:	17:0	17:.										
Sunday 24/09	15:00 - 15:50	15:50 - 16:00	16:00 - 16:40	16:40 - 17:05	17:05 - 17:30	17:30 - 20:00										
	Registration	Welcome Address	Martin Evans	Jakub Ślęzak	Ricardo Gutiérrez	Get Together										
Monday 25/09	09:00 - 09:40	09:40 - 10:05	10:05 - 10:30	10:30 - 11:00	11:00 - 11:40	11:40 - 12:05	12:05 - 12:30	12:30 - 14:00	14:00 - 14:40	14:40 - 15:05	15:05 - 15:30	15:30 - 16:00	16:00 - 16:40	16:40 - 17:05	17:05 - 17:30	
	Alberto Imparato	Fumika Suzuki	Jakub Zakrzewski	Coffee Break	Benjamin Lindner	Joël Mabillard	Benoît Mahault	Lunch Break	Raúl Toral	Yann Lanoiselée	Rick Bebon	Coffee Break	Juan P . Carbajal	Karol Capała	Shankar P . Das	
Tuesday 26/09	09:00 - 09:40	09:40 - 10:05	10:05 - 10:30	10:30 - 11:00	11:00 - 11:25	11:25 - 11:50	11:50 - 12:15	12:30 - 14:00	14:00 - 14:40	14:40 - 15:05	15:05 - 15:30	15:30 - 16:00	16:00 - 16:30	16:30 - 18:00		
	Francesco Caravelli	Paweł F. Góra	Jacek Polewczak	Coffee Break	Artem Ryabov	Nir Schreiber	Krzysztof Ptaszyński	Lunch Break	Aljaž Godec	Félix Ginot	Samuel Monter	Andrzej Fuliński	Coffee Break	Poster Session		
Wednesday 27/09	08:45 - 09:00	09:00 - 09:40	09:40 - 10:20	10:20 - 10:50	10:50 - 11:30	11:30 - 12:10	12:10 - 12:50	12:50 - 13:30	13:30 - 15:00	15:00 - 15:40	15:40 - 16:20	16:20 - 16:45	16:45 - 17:15	17:15 - 17:40	17:40 - 18:05	18:30
	Opening Speech	Hans-Rainer Trebin	Fernando Oliveira	Coffee Break	David Allender	Mikhail Osipov	Slobodan Žumer	Ewa Górecka	Lunch Break	Alberta Ferrarini	Holger Stark	Peter Palffy-Muhoray	Coffee Break	Piotr Kubala	Carmine Anzivino	Gala Dinner
Thursday 28/09	09:00 - 09:25	09:25 - 09:50	09:50 - 10:15	10:15 - 10:45	10:45 - 11:25	11:25 - 11:50	11:50 - 12:15	12:15 - 13:45								
	Krzysztof Kułakowski	Valentin Anfray	Piotr Garbaczewski	Coffee Break	lgor Sokolov	Arkady Pikovsky	Soheli Mukherjee	Lunch Break								