Nonequilibrium Dynamics of Micro- and Nanoparticles: Theory & Experiment

815. WE-Heraeus-Seminar

9 – 12 June 2024

at the Physikzentrum Bad Honnef, Germany



Introduction

The Wilhelm und Else Heraeus-Stiftung is a private foundation that supports research and education in science with an emphasis on physics. It is recognized as Germany's most important private institution funding physics. Some of the activities of the foundation are carried out in close cooperation with the German Physical Society (Deutsche Physikalische Gesellschaft). For detailed information see https://www.we-heraeus-stiftung.de

Aims and scope of the 815. WE-Heraeus-Seminar:

Nonequilibrium processes in chemistry, materials science and microfluidics are often based on motions of micro- and nanoparticles. In biology, these particles can be parts of a molecular machinery working inside living cells, bacteria, or other selfpropelled microorganisms. Studying nonequilibrium dynamics of micro- and nanoparticles in real-word systems and under well-controlled laboratory conditions is an active field of current research. Advancements of experimental techniques for tracking, trapping and manipulating particles together with high-resolution detection on microscopic time and length scales makes it possible to study motions with unprecedented precision on the level of individual particles.

This seminar discusses recent developments and new trends in nonequilibrium dynamics of micro- and nanoparticles. Major topics are dynamics of active particles in complex environments, unjamming of arrested particle motions in strongly disordered materials, dynamics out of liquids, effects of hydrodynamic interactions, emergent phenomena in transport across energy landscapes, driven motion in narrow pores, single-particle tracking and trapping, memory effects, and time-delayed feedback control.

The seminar aims to bring together leading scientists in the field to foster scientific advancements and to discuss steps for solving critical problems.

Scientific Organizers:

Prof. Philipp Maass	Universität Osnabrück, Germany E-mail: philipp.maass@uos.de
Dr. Artem Ryabov	Charles University, Czech Republic E-mail: artem.ryabov@mff.cuni.cz

Introduction

Administrative Organization:

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Registration	Elisabeth Nowotka (WE Herzeus Foundation)
	at the Physikzentrum, reception office Sunday (17:00 h – 21:00 h) and Monday morning

Sunday, 09 June 2024

17:00 – 21:00 Registration

18:00 BUFFET SUPPER and informal get-together

Monday, 10 June 2024

08:00	BREAKFAST	
08:45 – 09:00	Scientific organizers	Official Opening
09:00 – 09:45	Hartmut Löwen	Nonequilibrium dynamics of active colloids and polymers
09:45 – 10:30	Marjolein Dijkstra	From active Brownian spheres towards intelligent active polymers
10:30 – 10:35	Conference photo (in	the front of the lecture hall)
10:35 – 11:00	COFFEE BREAK	
11:00 – 11:45	Cynthia Reichhardt	Characterizing phase separation and critical behavior in active and driven matter with machine learning and noise power
11:45 – 12:30	Matthias Schmidt	Particles, functionals and symmetries
12:30	LUNCH	

Monday, 10 June 2024

14:00 – 14:45	Tetsuro Tsuji	Thermal force and hydrodynamic interaction characterized by optical force acting on micro- and nanoparticles
14:45 – 15:30	Pavel Zemánek	Nonequilibrium dynamics of levitated nanoparticles
15:30 – 16:00	COFFEE BREAK	
16:00 – 18:30	Poster Flash Presentat	ion and Poster Session
18:30	DINNER	

Tuesday, 11 June 2024

08:00	BREAKFAST	
09:00 – 09:45	Clemens Bechinger	Brownian particles in nonequilibrium baths
09:45 – 10:30	Roel Dullens	Geometric origin of particle and dislocation dynamics during grain boundary migration
10:30 – 11:00	COFFEE BREAK	
11:00 – 11:45	Alice Thorneywork	Interpreting fluctuations in a colloidal current
11:45 – 12:30	František Slanina	Hydrodynamic description of dense driven colloidal mixtures in narrow pores
12:30	LUNCH	

Tuesday, 11 June 2024

14:00 – 14:45	Anatoly Kolomeisky	Symmetry breaking of forward/backward transition times of single particles is determined by crowding, deviations from equilibrium and method of measurements
14:45 – 15:30	Yilong Han	Premelting-like phenomena in colloidal crystals and glasses
15:30 – 16:00	COFFEE BREAK	
16:00 – 16:45	Yael Roichman	The benefit of many stochastic searchers
16:45 – 17:00	Stefan Jorda	About the Wilhelm and Else Heraeus- Foundation
17:00 – 18:30	Free	
18:30	HERAEUS DINNER (Social event with cold	& warm buffet and complimentary drinks)
	Meeting with C. Kuttne Communications	r, Senior Editor of Nature

Wednesday, 12 June 2024

08:00	BREAKFAST	
09:00 – 09:45	Pietro Tierno	Emergent colloidal currents generated via exchange dynamics in a broken dimer state
09:45 – 10:30	Sabine Klapp	Self-assembly and self-organization in nonreciprocal anisotropic systems
10:30 – 11:00	COFFEE BREAK	
11:00 – 11:45	Frank Cichos	Feedback controlled active particles and liquids
11:45 – 12:30	Viktor Holubec	Delayed active matter
12:30 – 13:00	Scientific organizers	Poster Prize Ceremony and Closing
13:00	LUNCH	

End of the seminar and departure

NO DINNER for participants leaving on Thursday; however, a self-service breakfast will be provided on Thursday morning

Posters

Posters

Gursoy Bozkurt Akguc	Accumulation of nematic active particles on surfaces with free convection
Amy Altshuler	Starting over without forgetting the past
Gordei Anchutkin	Active particle steering in three dimensions
Alexander Antonov	 Colloidal transport in microfluidic Y-junctions Dynamics of active matter governed by Coulomb friction
Robin Bebon	Collective Hall current in chiral active fluids
Dima Boriskovsky	The fluctuation-dissipation relation holds for a macroscopic tracer in an active bath
Rémi Goerlich	Resetting as swift equilibration protocol in an
Sophie Hermann	Noether-constrained correlations and hyperforces in equilibrium liquids
Laura Hoek	Macroscopic piston-like active matter information engine
Jan Meibohm	Finite-time dynamical phase transitions in non- equilibrium relaxation
Michael Mekontchou Foudjio	Collective escape and homoclinic bifurcation phenomena in a nonlinear oscillators chain
Seemant Mishra	Fractional Shapiro steps in soliton-mediated driven particle transport across periodic energy landscapes
Kateřina Mladá	Lack-of-fit reduction in non-equilibrium thermodynamics applied to the Kac-Zwanzig model

Posters

Johanna Müller	Mathematical aspects of Noether's theorem in statistical mechanics
Vahid Nasirimarekani	Evaporation and micro-particle assembly inside an evaporating droplet; formation of flower-like pattern
Kristian Olsen	Dynamics of inertial particles under velocity resetting
Šimon Pajger	Jamming of active particles in quasi-1D geometries
Lisa Rohde	Hydrodynamic flow fields confine and polarise active particles around local heat sources
Florian Sammüller	Neural functionals in statistical mechanics
Sören Schweers	Scaling laws for single-file diffusion of hard rods with adhesive interactions
Andris Pavils Stikuts	Hydrodynamic viscous levitation of magnetically driven S- shape propellers
Ron Vatash	The benefit of many stochastic searchers. Many body resetting in colloidal suspension
Annika Vonhusen	Solitary cluster waves in periodic potentials
David Voráč	Delayed interactions in active matter models
Mateusz Wiśniewski	Effective mass approach to memory in non-Markovian systems
Fynn Wolf	Mechanical shape deformation of condensates through fibers
Zoe Talya Yagil	Thermodynamic uncertainty relation in driven colloidal suspensions

Abstracts of Talks

(In alphabetical order)

Brownian particles in nonequilibrium baths

Clemens Bechinger

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The power of thermodynamics comes at the expense of certain assumptions and idealizations. An important premise is the concept of a thermal bath in contact with the system under investigation. Typically, such baths are treated as an infinite reservoir of heat that remain in equilibrium regardless of whether the considered system is in equilibrium or not. Such description, however, is only valid when the relaxation time of the bath is much faster than typical time scales of the system. Otherwise, a driven system excites the bath out of equilibrium and thus interacts with nonequilibrium fluctuations. Experiments with externally or self-propelled colloidal particles suspended in viscoelastic baths whose relaxation times are on the order of seconds have revealed surprising phenomena that have no counterpart in viscous liquids. In my talk, I will discuss recent experimental findings including particle oscillations within moving optical traps, a fastened hopping dynamics across potential barriers, the strongly enhanced rotational diffusion of self-propelled particles, but also the occurrence of a surpising memory-induced Magnus force.

Feedback controlled active particles and liquids X. Wang¹ and F. Cichos¹

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Feedback control mechanisms are indispensable for technical and living systems to stabilize non-equilibrium states. In living systems feedback regulates biochemical processes, enhances sensory function, and allows for information transfer. It enables long range correlations and adaption or even evolutionary optimization.

We introduce soft matter feedback control by discussing experiments in which local dynamic temperature perturbations are used to manipulate the dynamics of fluids, macromolecules, or colloids through hydrodynamic boundary flows and thermophoretic drifts [1]. When the temperature perturbation is controlled by the current state of the sample, new dynamical functionality arises. Active colloids realized according to these principles and controlled in a feedback loop, for example, exhibit emergent nonlinear behavior. This nonlinear response and the accompanying memory provide a way to achieve information processing in synthetic active matter using active colloids as the nodes of an active physical reservoir [2]. We discuss the role of noise in this information processing system and other experimental realizations introducing intrinsic feedback processes.

- [1] Fränzl, M. & Cichos, F. Hydrodynamic manipulation of nano-objects by optically induced thermo-osmotic flows. *Nat Commun* **13**, 656 (2022).
- [2] Wang, X. & Cichos, F. Harnessing synthetic active particles for physical reservoir computing. *Nat. Commun.* **15**, 774 (2024).

From Active Brownian spheres towards Intelligent Active Polymers

<u>M. Dijkstra¹</u>

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In this talk, we show that the relaxation dynamics of self-propelled hard spheres accelerate by orders of magnitude upon increasing the activity [1]. Consequently, the glass transition shifts to higher packing fractions upon increasing the activity, enabling the examination of sphere packings with fluid-like dynamics close to random close packing. Expanding on these findings we explore their application in devitrifying glassy systems composed of mixtures of active and passive hard spheres [2]. Our simulations demonstrate that the crystallization of hard-sphere glasses can be significantly enhanced by introducing small amounts of active particles. Our findings offer a novel approach to fabricating crystalline materials from (colloidal) glasses. This is particularly important for materials that get easily kinetically trapped in glassy states, and when crystal nucleation hardly occurs. In addition, we show that grain boundaries can be removed in a polycrystalline material by the addition of active particles [3,4]. Finally, we study the collective behavior in a system of active Brownian spheres and active Brownian polymers with visual-perception-induced steering and alignment interactions. We find various dynamical structures like swarming, millings, and crystalline clusters.

- [1] R. Ni, M.A. Cohen-Stuart, M. Dijkstra, Nature Communications 4, 2704 (2013).
- [2] R. Ni, M.A. Cohen Stuart, M. Dijkstra and P.G. Bolhuis, Soft Mater 10, 6609 (2014).
- [3] B. van der Meer, L. Filion, and M. Dijkstra, Soft Mater 12, 3406 (2016).
- [4] B. van der Meer, M. Dijkstra and L. Filion, Soft Mater 12, 5630-5635 (2016).

Geometric origin of particle and dislocation dynamics during grain boundary migration

Roel P. A. Dullens

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Grain boundary (GB) migration induces significant changes in the structure of polycrystalline solids and has a pronounced effect on the macroscopic properties of these materials [1-3]. On the atomic scale, GB migration is governed a mechanism via which constituent particles are displaced between lattice sites of neighbouring grains. Despite many efforts to characterise such mechanism for GB migration, a comprehensive understanding of the migration mechanism in terms of the dynamics of atoms *and* dislocations remains largely unclear.

Here, we investigate this link between particle, defect and GB migration experimentally by using holographic optical tweezers [4] to create loop-shaped GBs in a model twodimensional colloidal crystal. We reveal a clear connection between the dynamics of particles and dislocations where local block rotations observed in the particle dynamics correspond to the reaction and glide of dislocations along the paths of maximum misfit. Hence, the paths taken by the dislocations correspond to regions of largest particle displacement. Moreover, we identify the particle dynamics to be guided by set of equivalence points between both lattices that act as points of transition as particles displace between grains. Using this geometric underpinning, we establish a framework that predicts the microscopic dynamics of particles and dislocations during GB migration in our two-dimensional crystals.

References

[1] JM Howe, Interfaces in materials. (John Wiley & Sons, 1997).

- [2] EO Hall, Proceedings of the Physical Society, Section B 64 (9), 747 (1951).
- [3] NJ Petch, Journal of the Iron and Steel Institute 174, 25 (1953).
- [4] FA Lavergne et al., PNAS 115 (27), 6922 (2018).

Premelting-like phenomena in colloidal crystals and glasses

X. Wang, B. Li, M. Li, Q. Zhang and Y. Han

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Analogous to premelting and prefreezing, are there other similar surface phenomena as a phase-transition precursor? Can premelting be generalized from crystals to amorphous solids? These questions could be asked and studied decades ago, but surprisingly have not been discussed in literature. We study these blind spots in material science using colloids with temperature-sensitive attractions.

We observe crystal surface premelting at the single-particle level for the first time [1] and find that monolayer and bilayer crystals exhibit distinct premelting and melting behaviors in experiment [1] and simulation [2]. Analogous to premelting and prefreezing, we propose the third type of surface wetting phenomenon as a phase-transition precursor and named it as pre-solid-solid transition, i.e. a surface polymorphic crystal formed before reaching the solid-solid transition [3]. We confirm it in colloid experiment (figure) and simulation [3], and attribute it to the lower-energy coherent interface. This thermal equilibrium behavior can also exist in nonequilibrium processes of melting, crystallization, and polycrystal annealing [3]. We suggested several atomic/molecular polymorphic crystals which may exhibit the pre-solid-solid transition. Glass melting lacks experiment at the single-particle level; Ultrastable glass has not been fabricated in colloids; Whether a glass can exhibit premelting has not

been explored. Our colloidal experiments address these three challenges and unveil two surface layers [4], based on our preliminary study about free surfaces of colloidal glasses [5]. As approaching the transition points, the thicknesses of the premelted surface liquid and pre-sollid-solid surface crystal all grow in power laws as predicted in premelting theory [4]. Similar behavior has been observed in polymer and molecular glasses, but it is called as surface mobile layer instead of premelting.



Figure: Pre-solid-solid transition in ref.[3].

- [1] B. Li, F. Wang, D. Zhou, Y. Peng, R. Ni, and Y. Han, Nature **531**, 485 (2016)
- [2] X. Wang, B. Li, X. Xu, and Y. Han, Soft Matter 17, 688 (2021)
- [3] X. Wang, B. Li, M. Li, and Y. Han, Nat. Phys. **19**, 700-705 (2023)
- [4] Q. Zhang, W. Li, K. Qiao, and Y. Han, Sci. Adv. 9, eadf1101 (2023)
- [5] X. Cao, H. Zhang, and Y. Han, Nat. Commun. 8, 362 (2017)

Delayed active matter

V. Holubec

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In many situations in science and engineering, finite speeds of signal transmission and processing affect the resulting behavior of the system. Usually, we describe such phenomena by stochastic processes with time delay. In this talk, I will first review the general features of delay stochastic differential equations [1-2]. Then I will present some consequences of instrumental time delay on steering artificial active Brownian particles [2-4]. Finally, I will discuss the influence of time-delayed interactions on critical scaling in the Vicsek model for bird flocks and insect swarms [5].

References

[1] V Holubec, A Ryabov, SAM Loos, K Kroy, Equilibrium Stochastic Delay Processes, NJP Physics **24**, 023021, 2022

[2] D Geiss, K Kroy, V Holubec, Brownian molecules formed by delayed harmonic interactions, NJP Physics **21**, 093014, 2019

[3] X Wang, PC Chen, K Kroy, V Holubec, F Cichos, Spontaneous vortex formation by microswimmers with retarded attractions, Nat. Commun. **14** (1), 56, 2023

[4] PC Chen, K Kroy, F Cichos, X Wang, V Holubec, Active particles with delayed attractions form quaking crystallites, EPL **142** (6), 67003, 2023

[5] V Holubec, D Geiss, SAM Loos, K Kroy, F Cichos, Finite-size scaling at the edge of disorder in a time-delay Vicsek model, PRL **127**, 258001, 2021

Self-assembly and self-organization in nonreciprocal anisotropic systems

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Recently much attention has been devoted to colloidal systems that are intrinsically out of equilibrium, a prime example being synthetic "active" colloids, but also colloids with non-reciprocal couplings (generated by a nonequilibrium environment) or colloids under feedback control. In this talk I will mainly address the impact of nonreciprocity, focusing on systems with anisotropic interactions. The first example concerns mixtures of repulsive active particles with non-reciprocal polar alignment, providing a minimal model of a system exhibiting both, clustering and polar ordering. We investigate the collective behavior of these systems using a combination of mean-field-like continuum theory, particle-based simulations of the underlying Langevin equations, and a corresponding fluctuation analysis [1,2]. We show that nonreciprocity has profound influence already below the threshold related to spontaneous time dependency of polarization dynamics. In particular, nonreciprocal alignment alone can induce asymmetrical density dynamics, where single-species clusters chase more dilute accumulations of the other species [2]. The second example is a system of passive colloids with field-induced interactions which, in equilibrium, form rigid clusters with extremely long live times [3]. By considering a binary version with asymmetric interactions, we show that nonreciprocity can have an annealing effect, allowing the system to escape kinetic traps yielding thermalization of clusters and even phase separation [4]. Finally, we make connection to another nonreciprocal nonequilibrium mechanism, that is, time-delayed feedback [5].

- [1] K. Kreienkamp and S.H.L. Klapp, New. J. Phys. 24 123009 (2022)
- [2] K. Kreienkamp and S.H.L. Klapp, arXiv:2403.19291, arXiv:2404.06305 (2024)
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- [4] S. Fariz Navas and S.H.L. Klapp, to be submitted
- [5] R. Kopp and S.H.L. Klapp, EPL 143 17002 (2023)

Symmetry breaking of forward/backward transition times of single particles is determined by crowding, deviations from equilibrium and method of measurements

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¹Rice University, Department of Chemistry, Houston, Texas, USA 77005 ² National Institute of Health, Bethesda, Maryland USA 20892

Microscopic mechanisms of natural processes are frequently understood by analyzing local particle transitions. Recent theoretical studies made a surprising discovery that in complex systems, the symmetry of molecular forward/backward transition times of single particles with respect to local bias in the dynamics may be broken and it may take longer to go downhill than uphill. The physical origins of these phenomena

remain not fully understood. We explore in more detail the microscopic features of the symmetry breaking in the forward/backward transition times by analyzing exactly solvable discrete-state stochastic models. It is found that the asymmetry in transition times depends on several factors that include how far is the system from equilibrium, the degree of particle crowding, the size of the system, as well as the methods of measurements of dynamic properties. Our theoretical analysis suggests that the asymmetry in transition times can be explored experimentally for determining the important microscopic features of natural processes by quantitatively measuring the local deviations from equilibrium and the degrees of crowding.

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- [2] J. Shin, A.M. Berezhkovskii and A.B. Kolomeisky, J. Phys. Chem. Lett. **11**, 4530–4535 (2020).
- [3] J. Shin, A.M. Berezhkovskii and A.B. Kolomeisky, J. Chem. Phys. 154, 204104 (2021).

Nonequilibrium dynamics of active colloids and polymers

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Active or activated colloids and polymers present valuable model systems to visualize nonequilibrium dynamics on micron length scales. Predictions of theoretical models can be directly compared to real-space experiments on colloids and bacteria. In this talk we shall discuss the dynamics of an active polymer in a porous matrix and show that the long-time diffusion coefficient can be largely tuned with an optimal geometric criterion stating that the run length of the particle equals roughly the geometric pore size [1]. We shall further address the case of dense entangled active polymer solutions and extract new scaling laws generated by activity [2]. Finally we consider magnetic colloids flowing through Y-junction channels and show – both by simulation of a model system and by experiment – the existence of a dynamical branching transition.

- [1] C. Kurzthaler, S. Mandal, T. Bhattacharjee, H. Löwen, S. S. Datta, H. A. Stone, Nature Communications **12**, 7088 (2021).
- [2] D. Breoni, C. Kurzthaler, B. Liebchen, H. Löwen, arXiv:2310.02929

Characterizing Phase Separation and Critical Behavior in Active and Driven Matter with Machine Learning and Noise Power

<u>C. J. O. Reichhardt¹</u>, C. S. Schimming¹, C. Reichhardt¹, and D. McDermott¹

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We examine motility-induced phase separation (MIPS) in two-dimensional run and tumble disk systems using both machine learning and noise fluctuation analysis. Our measures suggest that within the MIPS state there are several distinct regimes as a function of density and run time, so that systems with MIPS transitions exhibit an active fluid, an active crystal, and a critical regime. The different regimes can be detected by combining an order parameter extracted from principal component analysis with a cluster stability measurement. The principal component-derived order parameter is maximized in the critical regime, remains low in the active fluid, and has an intermediate value in the active crystal regime. We demonstrate that machine learning can better capture dynamical properties of the MIPS regimes compared to more standard structural measures such as the maximum cluster size. The different regimes can also be characterized via changes in the noise power of the fluctuations in the average speed. In the critical regime, the noise power passes through a maximum and has a broad spectrum with a 1/f^{1.6} signature, similar to the noise observed near depinning transitions or for solids undergoing plastic deformation. We extend a similar analysis to driven assemblies of superconducting vortices.

- [1] D. McDermott, C.J.O. Reichhardt, and C. Reichhardt, Phys. Rev. E **101**, 042101 (2020)
- [2] D. McDermott, C. Reichhardt, and C.J.O. Reichhardt, Phys. Rev. E **108**, 064613 (2023)

The benefit of many stochastic searchers Ron Vatash¹ and <u>Yael Roichman^{1,2}</u>

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Stochastic resetting involves randomly interrupting and then restarting a stochastic process. Its unique characteristics and the complexity of the phenomena it induces have attracted much attention. However, the rigorous exploration of resetting in many-body systems with interacting constituents remains unaddressed. Here, we study experimentally and numerically the impact of particle interactions on both global and local stochastic resetting of colloidal particles with optical tweezers. Using the renewal approach, we accurately predict the steady-state distribution in scenarios where we lack theoretical knowledge of the reset-free propagator (many-particle system) and in cases where we can analytically solve it (single particles). We quantify the effect of particle interactions on the emerging steady-state. For many searchers, resetting in beneficial only for a few searchers. Surprisingly, we find that local resetting outperforms global resetting significantly in a wide range of resetting rates.



Particles, Functionals, and Symmetries <u>Matthias Schmidt¹</u>, Sophie Hermann¹, and Florian Sammüller¹

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I describe recent progress in the statistical mechanics of systems of mutually interacting particles, as is relevant for modelling and understanding the behaviour of colloidal dispersions and more general soft matter. Many relevant structuring and transport phenomena in soft matter are accessible on the basis of particle-based simulation techniques. Much further insight can be gained through exploitation of a range of functional techniques [1-3]. (A functional is a map from a function to another function.) Classical density functional theory and its formally exact power functional generalization to nonequilibrium dynamics provide formally closed descriptions of the many-body physics under consideration [1]. The required functional relationships are thereby accessible via supervised machine learning [3,4]. While the data for training the neural networks that represent the neural functionals comes from simulations, the resulting computational efficiency allows for ease of application to multi-scale predictions with high accuracy. Neural functionals provide access to correlation functions via high-level programming on the basis of automatic differentiation and straightforward functional integration [3]. Exact Noether sum rules can thus be verified explicitly and used to carry out consistency and accuracy checks. The sum rules stem from applying Noether's theorem to the inherent symmetries of the statistical mechanics [2], which allows to systematically formulate and interrelate microscopically resolved force fields and force correlation functions [2,5]. Working with functionals is a very flexible approach, as is exemplified by the recent extension of classical density functional theory to arbitrary observables [6].

- 1. Power functional theory for many-body dynamics, M. Schmidt, Rev. Mod. Phys. **94**, 015007 (2022).
- 2. Why Noether's Theorem applies to Statistical Mechanics, S. Hermann & M. Schmidt, J. Phys.: Condens. Matter **34**, 213001 (2022) (Topical Review).
- Why neural functionals suit statistical mechanics, F. Sammüller, S. Hermann & M. Schmidt, J. Phys. Condens. Matter **36**, 243002 (2024) (Topical Review).
- Neural functional theory for inhomogeneous fluids: Fundamentals and applications, F. Sammüller, S. Hermann, D. de las Heras & M. Schmidt, Proc. Nat. Acad. Sci. **120**, e2312484120 (2023).
- 5. Noether-constrained correlations in equilibrium liquids, F. Sammüller, S. Hermann, D. de las Heras & M. Schmidt, Phys. Rev. Lett. **130**, 268203 (2023).
- Hyper-density functional theory of soft matter, F. Sammüller, S. Robitschko, S. Hermann & M. Schmidt, arXiv:2403.07845.

Hydrodynamic description of dense driven colloidal mixtures in narrow pores

F. Slanina

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Using a two-step mapping we describe the movement of dense suspensions of colloid particles interacting via steric repulsion. The mapping is equivalent to a hydrodynamic limit but involves a mean-field-like approximation This enables us to investigate the response of the ensemble of interacting particles on complex geometric constraints. Especially (but not only) we look at behavior of these particles in corrugated asymmetric channels, where ratchet effect and jamming are typical features. The approach can be directly generalized to multicomponent colloid systems, like mixtures of particles of different sizes, as well as to systems of active particles. In this talk, we also assess the precision of the hydrodynamic description by comparison with direct numerical simulations of mixtures of passive as well as active particles.

References

[1] F. Slanina and M. Kotrla, Phys. Rev. E **107**, 064606 (2023).

Interpreting fluctuations in a colloidal current

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The transport of molecules through biological and synthetic nanopores is governed by multiple stochastic processes that create noisy, fluctuating currents. Interpreting these fluctuations in experimental data provides a route to better understand transport mechanisms in nanoscale systems. Disentangling the effects of different noise generating mechanisms for molecular pores is, however, very challenging due to their inherent complexity and the short time and length scales associated with molecular dynamics. As such, colloidal models, which display analogous physical behaviour but are highly controlled and allow for visualisation of transport dynamics at the single particle level, offer valuable insights into confined transport processes.

Here, we study current noise experimentally at the single particle level by imaging colloidal particles driven through microfluidic channels by a difference in fluid pressure [1]. To draw a clear analogy with nanoscale transport studies, fluctuation behaviour is quantified by calculation of the power spectral density (PSD) – the correlation function most commonly used in this field. In dilute systems, currents fluctuate due to both the random arrival times of particles at and the distribution of particle speeds within the channel. This results in a characteristic form of the PSD and we show this can be modelled using expressions for shot noise with a finite transit time – a model borrowed from electronic circuit theory. Importantly, this also shows we can resolve experimentally the subtle differences in spectral scaling between non-equilibrium and equilibrium systems [2,3]. Finally, for high packing fractions of particles in the reservoir, we observe a suppression of fluctuations at low frequency. We link this to interparticle interactions in the reservoir, highlighting the importance of entrance mechanisms for transport through channels of finite length. We thereby demonstrate that our colloidal model can be used to establish concrete links between power spectral scaling and underlying mechanisms, making it an excellent platform with which to explore fluctuation behaviour in porous systems.

References

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[2] E. K. R. Mackay, et al., <u>arXiv:2311.00647</u> (2023)

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Emergent colloidal currents generated via exchange dynamics in a broken dimer state

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In this talk, I will describe a general strategy to assemble and transport polarizable magnetic microspheres in fluid media through a combination of confinement [1] and magnetic dipolar interactions [2]. We use a homogeneous magnetic modulation to assemble dispersed particles into rotating dimeric state and frustrated binary lattices and generate collective edge currents that arise from a novel, field-synchronized particle exchange process [3]. The observed, net bidirectional current is composed of colloidal particles which periodically meet assembling into rotating dimers, and exchange their positions in a characteristic, "ceilidh"-like dance. We develop a theoretical model that explains the physics of the observed phenomena as dimer rupture and the onset of current, showing agreement with Brownian dynamic simulations [4]. Further, we recently explore the transport of defects as non-magnetic inclusions in ferrofluids media and the anomalous dynamics of the broken/recombining dimers during the exchange process. Overall, we demonstrate an effective technique to drive microscale matter by using the interplay of steric confinement and dipolar forces, not based on any gradient of the applied field.

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Thermal force and hydrodynamic interaction characterized by optical force acting on micro- and nanoparticles

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Recently, optical trapping has been a useful common tool for manipulating the motion of small objects such as micro- and nanoparticles. In this talk, we present our recent experimental studies in which the optical trapping of micro- and nanoparticles are applied to the understandings of hydrodynamic forces acting on them.

The first part of the talk is devoted to the detection of thermal forces. When particles are dispersed in a fluid with inhomogeneous temperature field, they are known to move along the temperature gradient of the fluid: This nonequilibrium effect is called thermophoresis and its driving force is a thermophoretic force. One of the origins of the thermophoretic force is the counteraction of thermally-induced creeping flows, i.e., thermo-osmotic slip, along the surface of the particle. Here, we use the optically-trapped tracers confined around the target particle (Fig. 1(a)) to visualize the thermo-osmotic slip and show that this creeping flow is responsible for the thermophoretic force [1].

The second part of the talk will consider the role of hydrodynamic interaction between dispersed particles. The optical trapping of the particles using optical vortex beam confines them in a circular orbit centered at the laser focus. At the same time, the optical angular momentum drives the orbital motion of the particles (Fig. 1(b)). Here, we show experimentally that single particles exhibit a faint orbital motion but a significant speed up is achieved as the number of the particle in the orbit increases. This speed up is well explained by the Stokesian dynamics simulation and thus originated from the interparticle hydrodynamic interaction [2].



Fig. 1 (a) Schematic of the detection of thermo-osmotic slip [1] and (b) the speed up of the collrective orbital motion under an optical vortex beam [2].

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Nonequilibrium dynamics of levitated nanoparticles

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The recent experimental progress in control of the mechanical motion of a single levitated particle opens new ways to investigate more complex configurations in more dimensions or with more levitated and interacting objects. An optical levitation offers relatively easy tunability of the key system parameters (oscillating frequency, the strength of the optical coupling between particles, damping, effective temperature, etc.) over several orders of magnitude. Similarly, the forces acting upon the particles can be tuned between conservative and non-conservative, and various examples of nonequilibrium multidimensional dynamics can be demonstrated.

We provide a few experimental examples of nonequilibrium dynamics of a single optically levitated object with optically coupled degrees of freedom [1,2] and of more levitated objects where their optical coupling (referred to as optical binding) leads to the formation or synchronization of limit cycles [3,4]. Finally, we present a protocol of experimental amplification and squeezing of a motional state of an optically levitated nanoparticle in a stroboscopic sequence of switched potentials [5].

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Abstracts of Posters

(In alphabetical order)

Accumulation of nematic active particles on surfaces with free convection.

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This paper investigates the dynamics of nematic active Brownian particles on a disk surface under free convection flow. The study reveals the complex interplay between the particles and the flow, which alters the flow's symmetry and the aggregate's intensity and direction on the surface. The research highlights the changes in moment due to convective flow and particle scattering, along with broad contact interaction, which enable nematic particles to aggregate more efficiently than their spherical counterparts. The paper also discusses the potential to direct aggregation by adjusting flow rates.

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Starting over without forgetting the past

<u>Amy Altshuler^{1,2}</u>, Ofek Lauber Bonomo^{1,2}, Nicole Gorohovsky³, Shany Marchini³, Eran Rosen¹, Ofir Tal-Friedman^{3,2}, Shlomi Reuveni^{1,2}, and Yael Roichman^{1,2,3}

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In the past decade, resetting of random processes has been studied extensively, being relevant to natural processes. Under resetting, a random process can reach a stationary steady state that may reduce the average time it takes to reach a target. A resetting process generally includes cycles of a period of random motion followed by a period of return to the origin. When the random process is reset, the entire system starts from the same initial conditions as in the previous cycle. Inspired by scent trails left by ants, we study the case where the random motion leaves a mark on the environment. Namely, after resetting the system, the environment retains some memory of previously used paths. We implement this process using a self-propelled bristle robot moving within an arena filled with mobile obstacles. We return the bristle robot to the origin at constant time intervals. Surprisingly, we find that the propagator of motion is Gaussian in our experiments. We find that environmental memory increases the width of the steady state distribution. We observe that memory expedites the search in our setup.

Active particle steering in three-dimensions

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Synthetic active particles are a model system that mimics the self-propulsion of living matter to study fundamental aspects of non-equilibrium physics. Although various collective phenomena of synthetic active matter have been studied, virtually all experiments are performed in two dimensions. Hence, they show strong signatures of hydrodynamic and physicochemical effects related to substrate boundaries. Collective phenomena for synthetic active particles in 3 dimensions have not yet been experimentally investigated.

Here we introduce 3-dimensional control to the study of synthetic active matter. We demonstrate simultaneous control of thermophoretic microswimmers by single particle tracking in three dimensions using digital holography and darkfield pattern tracking. The thermophoretic swimmers are controlled by adaptive focusing using real-time spatial wavefront shaping. With the help of these experiments, we explore the interplay of thermophoretic propulsion, gravity, and optical forces for the active particles. The experimental realization of a three-dimensional active ensemble will provide new insights into the importance of surface boundaries for the collective behavior of active particles due to the altered topologies and collision probabilities in 3D.

Colloidal transport in microfluidic Y-junctions

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In microfluidics, the bifurcation of a microfluidic channel in the form of a letter "Y" (Yjunction) plays an important role due to its fundamental importance as a flow separator in complex networks. Recent developments in microscale design and microfluidics have suggested many ways to study the colloidal dynamics in such junctions through experimental methods. Here, we demonstrate through numerical simulations how the Y-junction controls the particle flow depending on their initialization in the system, interactions, and driving mechanisms. Our findings have also been validated in experiments where colloidal particles are driven by the fluid flow [1].

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Dynamics of active matter governed by Coulomb friction

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Coulomb friction, which is also known as dry friction, is a common phenomena that can be encountered in various systems where two solid surfaces are in contact and attempt to slide past each other. The friction force resists this relative motion and is almost independent of the relative velocity. We show that this characteristic feature of the Coulomb friction leads to emergence of mobility states when subjected to active, or self-propelled motion [1]. These dynamical states stems from the interplay between active forces propelling movement and frictional forces resisting it. When activity dominates over friction, we observe a super-mobile dynamical state, which reflects an anomalous scaling behavior of the diffusion coefficient with the active force.

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Collective Hall current in chiral active fluids

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Active fluids, composed of motile entities, have garnered enormous interest owing to the programmability of their collective spatiotemporal behavior that can be controlled by tuning physical properties at the individual level. We report a novel phase exhibited by locally aligning chiral active particles: (meta-)stable, dispersionless traveling bands that couple phase and mass transport. Intriguingly, bands are distinct from polar flocks since the particle current is neither parallel nor perpendicular to the direction of phase propagation, with magnitudes depending on the self-propulsion and angular speeds of particles. We thus report the first instance of a self-organized Hall (or Magnus) effect in chiral active fluids with a tunable Hall angle. Through particle-based simulations, we reveal the mechanism underlying this phenomenon and classify the emergence of bands by identifying the orbital radius of individual particle trajectories as dominant control parameter. While bands are (meta-)stable for small to intermediate

radii, rare density fluctuations can lead to the rupture of bands and induce a crossover to the linearly-stable synchronized state. This effect is amplified for larger orbital radii and we uncover a discontinuous transition at a critical radius, beyond which bands are no longer observed. We corroborate our results by deriving a minimal hydrodynamic theory through coarsegraining the microscopic equations of motion. Within this framework we show that bands arise as nondispersive soliton solutions that fully account for the properties observed in simulations.



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The fluctuation-dissipation relation holds for a macroscopic tracer in an active bath

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The fluctuation-dissipation relation (FDR) links thermal fluctuations and dissipation at thermal equilibrium through temperature. Extending it beyond equilibrium conditions in pursuit of broadening thermodynamics is often feasible, albeit with system-dependent specific conditions. We demonstrate experimentally that a generalized FDR holds for a harmonically trapped tracer colliding with self-propelled walkers. The generalized FDR remains valid across a large spectrum of active fluctuation frequencies, extending from underdamped to critically damped dynamics, which we attribute to a single primary channel for energy input and dissipation in our system.



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Driven force formation of the microfluidics cylindrical pores and its networks at interfaces of SS321/Zr1Nb bimetal system

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The report presents a result on the finding of the cylindrical micropores and its networks formation at interfaces of "StainlessSteel321/Zr1Nb-alloy" bimetal system (SS321) solid-state joined with an interlayer of Cu/Nb. A formation of the pores and its enrichment in such impurity as S, Cl, Ti occurs simultaneously. In turn, the 2D impurity enrichment contrasts elucidate a fact of the microstructures formation. SS321/Zr1Nb system was obtained using vacuum hot rolling. A part of the rolled sheet was also subjected to simultaneous thermal and mechanical cycling at 350 grad. C. Such microanalytical techniques as SEM EDX, micro-PIXE and -IBIEBS, -SIMS were applied to study microstructure and element concentration composition of bimetal system interfaces. SEM EDX and micro-SIMS were performed in line scan mode, micro-PIXE and -IBIEBS – 2D element concentration mapping one. Lengths, diameters, details of walls of the micropores were explored as well as its impurity concentration distributions, 2D details of micropore networks at Cu interlayer. It was concluded that pore's microstructures formation has microfluidics nature. It was also supposed a pore's formation driven force origin. A potential application of the observed microfluidics processes during solid-state joining and its subsequent microstructures relaxation at the welded interfaces will also be discussed in the report.

Предлагается следующий сценарий формирования микропор и сети из них. При горячей прокатке в вакууме при температурах около ??? град.Цельсия и при термомеханическом циклировании возможны следующие физико-химические процессы в интерфейса биметаллической системы "StainlessSteel321/Cu/Nb Zr1Nb-alloy" (SS321/Cu/Nb/Zr1Nb): i) интенсивные диффузионные процессы компонентов системы и загрязняющих микропримесей (S- [трибодиффузия и ссылка], Н [коэф.дифф. в меди и стали и предел растворимости], Ті (основной легирующий элемент в стали SS321, но загрязняющая примесь в прослойке из меди), О (элемент адсорбированной воды или в составе более сложной поверхностной загрязняющей пленки); іі) образование волнистого рельефа на границе раздела «сталь-медь» и концентрация таких примесей как S, H, Ti, O (микро-ХРИ) с выделением преципитатов новой фазы (SEM-микрофотография); ііі) микровзрывы (пирофорный эффект) таких микрочастиц как Fe, Ni, Mn, Ti, TiO, Fe2S и других возможных более сложных по микроструктуре и химической формуле выделений новой фазы; iv) во время и/или при остывании факела возможно интенсивное течение паров газов в цилиндрической полости в расплаве меди; v) остывание полостной микроструктуры с образованием тонких стенок из сульфида меди (micro-IBIEBS, -PIXE), vi) эффект, обратный растворимости микропримесей (S, Cl, Ti, к примеру). Следует отметить, что при микровзрыве микрочастиц, содержащих в своем составе микропримеси титана и распределенных в слое стали вблизи границы раздела «сталь-медь», не наблюдается эффекта «остывшего факела» или «микрокумулятивной струи» двумерной или микрокометы» «хвоста ПО картинке распределения микроконцентаций серы в «остывшем факеле»

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Resetting as swift equilibration protocol in an anharmonic potential

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We present [1] and characterize a method to accelerate the relaxation of a Brownian object between two distinct equilibrium states. Instead of relying on a deterministic time-dependent control parameter b(t) governing the potential acting on Langevin trajectories (Fig. **a**, [2]), we use stochastic resetting (Fig. **b**, [3]) with time-dependent rate $\lambda(t)$ to guide and accelerate the transient evolution. The protocol is investigated numerically, and its thermodynamic cost is evaluated with the tools of stochastic energetics. Remarkably, we show that stochastic resetting significantly accelerates the relaxation to the final state (Fig. **d**) with respect to a standard potential quench (Fig. **c**). This stochastic protocol exhibits energetic and temporal characteristics that align with the scales observed in previously investigated deterministic protocols [2]. Moreover, it expands the spectrum of stationary states that can be manipulated, incorporating new potential profiles achievable through experimentally viable protocols.



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Noether-constrained correlations and hyperforces in equilibrium liquids

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Noether's calculus of invariant variations in statistical mechanics yields exact identities ("sum rules") from functional symmetries. The invariance of spatial transformation of the underlying classical many-body Hamiltonian at first order in the transformation field Noether's theorem yields the local force balance. At second order three distinct two-body correlation functions emerge, namely the standard two-body density, the localized force-force correlation function, and the localized force gradient. An exact Noether sum rule interrelates these correlators [1]. More generally exploiting invariance of a thermally averaged classical phase space functions results in hyperforce sum rules [2]. These relate the mean gradient of a phase-space function to its negative mean product with the total force. Both global and locally resolved identities hold and similar to Hirschfelder's hypervirial theorem, the hyperforce sum rules apply to arbitrary observables in equilibrium. As applications we investigate via computer simulations (including Lennard-Jones, Yukawa, soft-sphere dipolar, Stockmayer, Gay-Berne and Weeks-Chandler-Andersen liquids, monatomic water and a colloidal gel former) the emerging one-body force fluctuation profiles in bulk and confined liquids [1,2]. These local correlators quantify spatially inhomogeneous self-organization, demonstrate their fundamental role in the characterization of spatial structure and their measurement allows for the development of stringent convergence tests and enhanced sampling schemes in complex systems.

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Macroscopic Piston-Like Active Matter Information Engine

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The second law of thermodynamics states that the entropy of an isolated system cannot decrease. The famous paradox of Maxwell's daemon highlighted that if information is gathered on the system subsequent feedback can cause entropy reduction without direct work input. Based on this idea, information engines use measurement and feedback to extract work from a system. We study a specific configuration of an information engine that is similar to a piston compression setup. We monitor active particles moving in a closed system with one boundary functioning as a movable piston. Whenever the area near that wall is vacant, we move the wall to compress the particles making sure the wall does not apply any external forces. Studying a 2D arena and self-propelled bristle-bots as particles, our aim is to examine the unique characteristics arising when the system inherently operates far outside of thermodynamic equilibrium. To do so, we measure, under quasi-static conditions, the information gained by the engine, the work output obtained through its operation, and subsequently evaluate its efficiency.

Preliminary results show that more work can be extracted from an information engine operated by active particles. Moreover, while in equilibrium the most efficient protocol for compression follows a relatively simple formula dependent mostly on the probability that compression is possible, our results show that far from equilibrium a more complex optimization process must be applied to achieve maximal efficiency.

Finite-time dynamical phase transitions in nonequilibrium relaxation

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This poster gives an overview over a recently discovered class of phase transitions, so-called finite-time dynamical phase transitions¹⁻³. These transitions occur in the extreme-event statistics of relaxing systems in non-equilibrium statistical mechanics.

Finite-time dynamical phase transitions appear in the transient relaxation of dissipative single and many-body systems after an instantaneous quench of the environment. The simplest example is a single, e.g. colloidal, particle in a double well potential at weak noise, subject to an instantaneous quench of the potential to a single well. During the transient relaxation, the rare-event statistics of certain observables exhibit singular points, i.e., kinks. These kinks are the consequence of sudden switches in the most likely rare-event dynamics^{1,2}, the optimal fluctuations, and they occur at sharp, finite times, so-called critical times.

The poster explains how the kinks and switches correspond to dynamical phase transitions, whose control parameter is time, as opposed to non-dynamical external parameters such as temperature or pressure. The interpretation as phase transitions proves to be fruitful, because established concepts from equilibrium and non-equilibrium statistical mechanics can be used to identify and classify the transitions.

For lattice-based models, finite-time dynamical phase transitions exhibit critical fluctuations, with non-mean-field critical exponents⁴. A careful finite-size scaling analysis enables one to extract these.

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Collective escape and homoclinic bifurcation phenomena in a nonlinear oscillators chain

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The phenomenon of deterministic collective escape of particles from the cubic on-site potential well in the presence of both uniform damping and a periodic force is studied. Using analytical techniques such as the separation of time and space as well as the Melnikov theorem, the condition on the periodic force for which a single particle exhibits an irregular motion induced by the homoclinic bifurcation (HB) is derived. Numerical simulation showed that this irregular motion can lead to a strong localization of energy on all the coupled particles allowing them to collectively cross the energy barrier. Moreover, the critical value of the driving force inducing collective escape increases as the potential energy barrier increases and decreases as its frequency increases. Depending on the frequency range of the driving frequency, the collective escape and HB can occur simultaneously; otherwise, the HB prevails.

Fractional Shapiro steps in soliton-mediated driven particle transport across periodic energy landscapes

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Applying both a DC and AC current to a Josephson junction results in a step-like shape of the current-voltage characteristics. Analogues of these so-called Shapiro steps have been observed for colloidal particles driven across periodic optical energy landscapes by a constant drag plus a time-periodic force: when the drag force is increased, the mean particle velocity stays constant in certain intervals, where the mean velocity equals integer multiples of the product of the driving frequency and the wavelength of the periodic potential [1, 2]. Non-integer, fractional Shapiro steps are commonly found for single-particle transport in periodic landscapes different from a sinusoidal one. We present a semi-analytical theory to explain the occurrence and to quantify features of these fractional steps. Interestingly, fractional Shapiro steps are obtained also when driving highly crowded systems of hard spheres across periodic energy landscapes, where solitary cluster waves mediate particle transport [3-5]. We explain this effect by introducing an effective periodic potential for the collective soliton dynamics.

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Lack-of-fit reduction in non-equilibrium thermodynamics applied to the Kac-Zwanzig model <u>Kateřina Mladá</u>¹, Martin Šípka² and Michal Pavelka²

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Microscopic particle dynamics is purely reversible, yet when observed macroscopically, irreversible evolution occurs. How does the irreversibility emerge? On the example of Kac-Zwanzig model, we show the emergence of irreversible behavior out of a purely reversible Hamiltonian dynamics, caused only by the reduction of observed degrees of freedom. Furthermore, the irreversible evolution is found as a sum of Hamiltonian and gradient dynamics. This is done using the so-called lack-of-fit reduction.

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Mathematical Aspects of Noether's Theorem in Statistical Mechanics

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Noether's Theorem of invariant variations forms a staple of modern physics. In standard applications the theorem connects symmetries of the action functional of a given physical system with conservation laws. In recent developments Noether's Theorem was used in various different ways in the Statistical Mechanics of manybody systems. Thereby exploiting invariances of central statistical functionals, such as the partition sum, the free energy density functional, and the nonequilibrium power functional, led to a range of results. These include newly derived exact identities as well as a categorization of existing statistical mechanical sum according to the Noetherian concepts [1-3]. In the present contribution various mathematical properties of the thermal invariance shifting operation on the classical phase space of many-body systems that underlies the variational techniques are discussed [4].

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Evaporation and micro-particle assembly inside an evaporating droplet; formation of flower-like pattern Vahid Nasirimarekani¹

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Pattern formation is a phenomenon involved in many different aspects of life on our planet. Fluids, as an abundant phase in nature and in which life has formed, host many active and non-active particles that exhibit various patterns. The droplet form of a fluid undergoing evaporation is a non-equilibrium system that results in remarkable pattern formation, which can be controlled by the chemistry of the droplet and external physical factors. Here, I have observed a unique flower-like pattern formation of micron sized particles inside an evaporating droplet containing salt and surfactant. The interaction of salt with the surfactant was seen to induce strong local gradient flows that resulted in the formation of radially formed regular flower-like petals. These experiments suggest the importance of surfactant-driven flow in biological samples, which can be useful for understanding the pattern formation of biological components.

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Dynamics of inertial particles under velocity resetting

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Transport processes that exhibit intermittent dynamics is ubiquitous in Nature, ranging from micro-scale processes where collisions with a disordered environment induces loss of momentum, to behavioural patterns in macroscopic active matter systems where stop-and-go locomotion is common motility strategy. Using a stochastic resetting framework, we model intermittent stops by resetting events of the velocity variable, while the position remains unaffected by the reset. Based on a renewal equation for the full phase-space propagator, we derive general expressions for late-time transport coefficients which are valid for any underlying (e.g. reset-free) system. Such velocity resetting generally results in a linearly growing mean squared displacement at late times. A non-trivial dependence on the rate may appear due to multiple timescales and crossovers in the reset-free dynamics. An extension that incorporates refractory periods after each reset is considered, where post-resetting pauses can lead to anomalous diffusive behaviour. Our framework may also be of relevance to other systems where resetting only affects a subspace of a higher-dimensional phase space.

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Jamming of active particles in quasi-1D geometries <u>Š. Pajger</u>¹

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We study the behavior of active particles in 1D simple exclusion process-like models, where on single sight there can be at most two particles. In particular, we also study a case with a broken spatial symmetry, where in one direction there are dead-ends, in which active particles can be trapped. We investigate in detail the jamming transition, i.e. when a situation occurs, in which most of the particles are in one cluster and cannot move, and how such a cluster behaves. We show that the jamming transition is of first-order type, characterized by long-lived metastable states.

Hydrodynamic flow fields confine and polarise active particles around local heat sources

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Many biological components on the microscale use activity and self-propulsion in order to form functional structures. In these nonequilibrium processes, they interact with the environment by responding to temperature and composition gradients or to flow fields. These self-organization principles are transferred to artificial active particles, which act as model system to mimic biological motors, but yet have only limited functionality.

Here, we expose self-thermo-phoretic Janus particles to an environment with tunable hydrodynamic flow and temperature fields. A heated paramagnetic silica particle acts as a heat source and generates a thermo-osmotic flow field due to a temperature gradient on the substrate. The control of temperature in our sample enables us to locally change the generated hydrodynamic flow field. We study the translational and orientational dynamics of the Janus particles relative to the heat source depending on temperature and laser intensities. The interplay of the local hydrodynamic flows with the activity of the Janus particles results in a potential that confines the Janus particles to a structure around the heat source with a fixed distance and orientation to it. We thus find a polarisation of the Janus particles that align with the flow field.

Neural functionals in statistical mechanics

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Classical density functional theory and power functional theory provide formally exact frameworks for the description of many-body systems in and out of equilibrium. However, concrete applications are often held back by the difficulty of finding the underlying functional relationships. I will show how machine learning can be utilized effectively in these theories in order to investigate the behaviour of inhomogeneous fluids and soft matter. Neural networks act as precise and flexible representations of the central functional maps and they are trained with many-body simulation data, see Figure 1. These neural functionals facilitate straightforward predictions which supersede state-of-the-art analytic treatments in accuracy [1]. Successful applications include multiscale problems such as colloidal sedimentation under gravity and the inverse design of colloidal transport [2]. The neural functionals further allow for the implementation of a stand-alone theoretical framework, which provides access to a multitude of related quantities of interest with unprecedented computational efficiency. The neural functional theory thereby gives insight into the structural and thermodynamic properties of a fluid [3], as becomes particularly relevant for investigating liquid-gas phase separation and critical phenomena. Additionally, neural functionals support a recent exension of classical density functional theory for incorporating arbitrary observables, which makes complex order parameters such as cluster statistics accessible via hyper-density functionals [4].



Figure 1: Neural functional workflow

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Scaling laws for single-file diffusion of hard rods with adhesive interactions

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Single-file motion of particles occurs in narrow channels when particles cannot pass each other. We study how single-file diffusion is affected by adhesive interaction as described by Baxter's model of sticky hard spheres [1]. To simulate this process, a new method for modeling Brownian motion based on the dynamics of particle clusters is developed [2]. We find that the adhesive interaction slows down normal diffusion at short times and speeds up subdiffusion at long times. We reason this behavior by setting up a scaling theory that provides a full description of the timedependent mean-squared displacement of a tagged particle [3]. The theory is in excellent agreement with the simulated behavior. Both the slow-down of normal diffusion and the speed-up of subdiffusion are caused by particle clustering induced by the adhesive interaction. The enhancement of subdiffusion can be quantified in measurements irrespective of how tagged particles are injected into the system.

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Hydrodynamic viscous levitation of magnetically driven S-shape propellers

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Hydrodynamic interactions (HIs), namely solvent-mediated long-range interactions between dispersed, microscopic particles, play a crucial role in the emergent dynamics of many active systems, from swimming bacteria to swarms of propelling microrobots. For example, HIs forces the bacteria E. Coli tend to swim close to a surface, where it performs a circular trajectory nearby [1,2,3]. The attraction results from the pusher type force dipole of the bacteria, which creates a flow field able to force the bacteria towards the wall [4]. Similarly, for a puller type swimmer, the generated flow field induces a repulsion from the wall. However, for pullers, the alignment parallel to the wall is not a stable configuration. Inspired by this effect, we have designed a microscale magnetic rotor able to produce a puller-like force dipole, but with a stable alignment parallel to the wall.

These S-shape lithographic particles are doped with nanoscale magnetic colloids and can be manipulated via external, time-dependent magnetic fields. Under a rotating, circularly polarized magnetic field, these propellers are subjected to a magnetic torque, and rotate exerting a force on the surrounding fluid. Because of the anisotropy of the drag coefficient on the elongated shape, similar to a pusher type bacterium, a pair of forces arise pointing towards the center of mass of the particle. Since the S-shape rotates above a wall, it experiences a lift force directed upward. We optimize the shape of the S particle to get the greatest lift force. Since the lift force decreases with the distance from the wall, we can calculate the equilibrium rotation height for different rotation frequencies. We find that an S-shaped particle with the cross-section radius of 3 microns and the length of 120 microns lifts to a height of around 100 microns when rotated at a frequency of 6 Hz in water-glycerol mixture with the viscosity 9.7 mPa s.

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The benefit of many stochastic searchers

Many body resetting in colloidal suspension

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Abstract

Stochastic resetting involves randomly interrupting and then restarting a stochastic process. Its unique characteristics and the complexity of the phenomena it induces have attracted much attention. However, the rigorous exploration of resetting in many-body systems with interacting constituents remains unaddressed. Here, we study experimentally and numerically the impact of particle interactions on both global and local stochastic resetting of colloidal particles with optical tweezers. Using the renewal approach, we accurately predict the steady-state distribution in scenarios where we lack theoretical knowledge of the reset-free propagator (many-particle system) and in cases where we can analytically solve it (single particle system). We quantify the effect of particle interactions on the emerging steady-state. For many searchers, resetting is beneficial only for a few searchers. Surprisingly, we find that local resetting outperforms global resetting significantly in a wide range of resetting rates.

Solitary cluster waves in periodic potentials

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Recent theoretical and experimental studies of driven Brownian motion of hard spheres [1] showed that cluster-mediated transport in one-dimensional periodic potentials can proceed in form of solitary waves [2,3]. We present a theory [4] that predicts the minimal number of particles needed for soliton formation, the number of solitons at larger particle numbers, soliton velocities and soliton-mediated particle currents. It moreover allows to understand effective repulsive soliton-soliton interaction seen in measurements. The theory is developed for a sinusoidal potential and tested for other periodic potentials.

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Delayed interactions in active matter models

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

Here, we investigate the applicability of spin-wave approximation to particle active matter models featuring delays. These models include the Vicsek and the more recent Inertial Spin Model (ISM) [1], neglecting and considering the orientational inertia. Our work introduces two levels of spin-wave approximation: discrete network and the continuum limit. The Vicsek model shows a good agreement with both types of approximation, provided that local perturbations remain within certain bounds. Conversely, the ISM exhibits satisfactory agreement only at the network level. Our findings represent a step towards a comprehensive hydrodynamic theory for delayed active many-particle models.

Effective mass approach to memory in non-Markovian systems

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

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Mechanical shape deformation of condensates through fibers

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Biomolecular condensates are a much-studied current topic of interest. They are membraneless organelles within the cell or the nucleus which typically consist of DNA/RNA and protein [1]. Despite different compositions, a unifying principle underlying their formation is the importance of multi-valent interactions between the constituent components [2,3]. Biomolecular condensates range from liquid to gel or even mature to become fibrils. Due to energy minimization, liquid condensates typically take on a spherical shape. However, several studies have shown that some liquid-like droplets can exist in different shape configurations [4,5]. One possible mechanism for these complex shapes is due to the interplay between the components of the droplets and fibers such as actin or tubulin, FXR1 or FUS fibrils. In this work, we use coarse-grained molecular dynamic simulations to study the formations of several possible morphologies, including lens and tactiod shapes [4]. We believe a determining factor will be the ratio of fiber length to condensate radius in equilibrium as well as the bending rigidity of the fibers. Further, we hope to capture the dynamics of how the fibers are incorporated into the condensate as well as how they organize. The insights acquired through the simulations will hopefully further our understanding of the functionality behind the deformations.

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Thermodynamic Uncertainty Relation in Driven Colloidal Suspensions

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The Thermodynamic Uncertainty Relation (TUR) establishes a fundamental limit on the measurement precision of a thermodynamic current in a system out of equilibrium. This limit is linked to the system's dissipation rate, traditionally quantified by entropy production. Recent research suggests alternative dissipation measures that could provide tighter bounds for strongly driven systems.

We investigate the tightness of these different bounds by studying the TUR in a steady-state driven colloidal suspension. Our experiment involves a single colloidal particle driven in a circular path, creating rotational flow with a radial decay proportional to r^{-4} . This setup allows us to explore a wide range of driving strengths (represented by the Péclet number, Pe) spanning three orders of magnitude.

Our findings reveal a characteristic dependence of the TUR on the driving force. We normalize the TUR with the diffusion coefficient and mean velocity to identify scaling behavior. By comparing our results to the existing bounds, we aim to identify the conditions under which each bound offers the tightest constraint.