DY 42: Poster: Active Matter, Soft Matter, Fluids

Time: Thursday 13:00–16:00 Location: P1

DY 42.1 Thu 13:00 P1

Transition to mesoscale turbulence in an active fluid — •Henning Reinken[1], Sebastian Heidenreich[2], Markus Bär[2], and Sabine H.L. Klapp[1] — [1]Technische Universität Berlin — [2]Physikalisch-Technische Bundesanstalt

Microwsimmer suspensions, a paradigmatic example of an active fluid, self-organize into complex spatio-temporal flow patterns, including regular vortex lattices and mesoscale turbulence, a highly dynamical state that exhibits a characteristic length scale. This work investigates the transition to this turbulent state using a continuum-theoretical approach for the effective microswimmer velocity field [1], where the dynamics is governed by the competition between relaxation to a regular vortex lattice and destabilization by nonlinear advection. For the unconstrained bulk flow, we show how to identify the onset of mesoscale turbulence analytically. To this end, we determine the linear stability of the vortex lattice state by explicitly taking into account the coupling between multiple modes via the nonlinear terms. Recent experiments [2] have also demonstrated how vortex lattices can be stabilized by small obstacles [3]. Using the continuum-theoretical approach, we further show numerically that the formation of these patterns exhibits features of a continuous second-order equilibrium phase transition in the 2D Ising universality class [4].

[1] Reinken et al., Phys. Rev. E **97**, 022613 (2018)
[2] Nishiguchi et al., Nat. Commun. **9**, 4486 (2018)
[3] Reinken et al., Commun. Phys. **3**, 76 (2020)
[4] Reinken et al., Phys. Rev. Lett. **128**, 048004 (2022)

DY 42.2 Thu 13:00 P1

Dynamics and clustering of active run-and-tumble particles on two-dimensional lattices — •Lars Torbjørn Stutzer and Peter Sollich — Institut für Theoretische Physik, Georg-August Universität Göttingen

We study the dynamics of run-and-tumble particles on two-dimensional lattices, focusing on the effects of lattice geometry (square, triangular and hexagonal) and maximum occupation number $n_{\max}$ per lattice site. We identify three phases in the stationary state: a cluster (C) phase with extensive clusters formed by motility-induced phase separation, which appears only for $n_{\max} \geq 2$; a gas (G) phase consisting of finite-sized clusters; and a new sponge (S) phase where small fluctuating clusters percolate. The nature of the transitions between these phases depend on lattice type and density. C-G transitions are mostly, but not always, first order, while C-S transitions are continuous. Single particle displacement distributions become non-Gaussian at higher densities, with intermediate exponential tails. Considering finally the transient dynamics from a random initial condition, the time it takes for clustering to appear in the system is independent of the tumble rate α but grows with the lattice coordination number and (exponentially or stronger) with $n_{\max}$.

DY 42.3 Thu 13:00 P1

Pressure in inertial active particle systems with frictional contacts — •Kay-Robert Dormann, Lukas Hecht, and Benno Liebchen — Institut für Physik kondensierter Materie, Technische Universität Darmstadt, Hochschulstr. 8, 64289 Darmstadt, Germany

In systems of isotropic overdamped active Brownian particles (ABPs), the pressure is a state function [1]. It can be shown, that an equation of state (EOS) also exists, if the ABPs are inertial [2]. Here, we explore inertial active Brownian particles [3,4] with additional frictional contacts and find that no EOS exists. We attribute this to the fact that the rotational diffusion depends on density in the presence of frictional contacts.

The breakdown of the EOS due to frictional contacts has interesting implications: for example, when embedding a passive Janus-sphere, whose two hemispheres show a different stiffness, into an active bath, the sphere shows active Brownian motion. In addition, we find that frictional contacts and the associated breakdown of the EOS also have interesting implications for motility-induced phase separation as we will specify on the poster.

[1] A. P. Solon et al., Phys. Rev. Lett. 114, 198301 (2015).
[2] Y. Fily et al., J. Phys. A Math. Theor. 51, 044003 (2018).
[3] S. Mandal et al., Phys. Rev. Lett. 123, 228001 (2019).
[4] L. Hecht et al., Phys. Rev. Lett. 129, 178001 (2022).

DY 42.4 Thu 13:00 P1

Advanced Sampling Methods for Non-Equilibrium Particles — •Thomas Kiechl, Michele Caraglio, and Thomas Franosch — Institute for Theoretical Physics, Universität Innsbruck, Innsbruck, Austria.

Active particles or microswimmers are capable of converting energy into directed motion - which is why they are classified as out-of-equilibrium systems. Microswimmers, such as bacteria or spermatozoa often find themselves in a *target search* situation, where the microswimmers have to make a transition from an initial area to a target area crossing complex environments. Transition Path Theory, a rigorous statistical mechanics description of transition processes, can be generalized to characterize the target search problem. A simple way of modeling a complex environment for the microswimmer is via an external potential, in which the metastable initial position is separated from the target by an energy barrier. This makes the target search a *rare event*, in which the timescales of the fluctuations in the metastable states and the transition process are separated. Brute force simulations solving the equations of motion are inefficient due to this gap in timescales. The main result is that a more efficient sampling method, Transition Path Sampling (TPS), originally developed for rare transitions of passive systems, can be generalized to Run-and-Tumble systems. TPS is a Monte Carlo simulation of successful trajectories where the new trajectory is accepted according to a metropolis rule based on a path integral formulation.

DY 42.5 Thu 13:00 P1

Markov state modelling of self-assembling active triblock Janus particles — •Salman Fariz Navas, Juri Schubert, and Sabine H.L. Klapp — ITP, Technische Universität Berlin, Germany

Active triblock Janus particles have been shown to form open-cell colloidal lattices in both experiments as well as simulations. Such structures are of particular interest owing to their novel optical and mechanical properties. However, the self-assembly of open-cell lattices is a multistep process involving the formation of many intermediate competing structures resulting in long time-scales.

Here, we develop a Markov State Model for a self-assembling active triblock Janus particle system [1] from particle resolved Brownian Dynamics simulations by reducing the continuous many particle dynamics into a discrete set of states [2],[3]. We use the local order parameters introduced in [4] to develop the discrete states. The transition probability matrix between these states can then be constructed using which, information regarding the metastable states, the relaxation times and the pathways relevant to the aggregation process can be extracted.

[1] S. A. Mallory and A. Cacciuto, J. Am. Chem. Soc. 141, 2500 (2019).
[2] J.-H. Prinz, H. Wu, M. Sarich, B. Keller, M. Senne, M. Held, J. D. Chodera, C. Schütte, and F. Noé, J. Chem. Phys. 134, 174105 (2011).
[3] S.F. Navas and S.H.L. Klapp, in preparation.
[4] H. Eslami, P. Sedaghat, and F. Müller-Plathe, Phys. Chem. Chem. Phys. 20, 27059 (2018).

DY 42.6 Thu 13:00 P1

Dynamics of an active agent subject to orientational resetting — •Yanis Baouche and Christina Kurzthaler — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

We study the dynamics of an active particle whose swimming direction is subject to rotational diffusion and a stochastic resetting mechanism. The latter allows for taking into account the particle's response to external stimuli.

We use renewal processes to model the reorientation mechanism of the active agent and provide analytical expressions for the characteristic function of the stochastic process and its low-order moments.

Finally, the interplay between rotational diffusion and resetting of the particle's orientation is quantified for different resetting distributions.

DY 42.7 Thu 13:00 P1

Adaptive microvascular remodeling under flow — Fatemeh Mirzapour-Shafiyi, •Leonie Karr, and Karen Alim — School of Natural Sciences, Technische Universität München

Vessel morphology is adapted to minimise energetic costs of dissipation

and homogenize flow transport in the network. Resource-deprived tissues produce chemotactic agents to induce vessel formation during development and in tissue homeostasis. The primitive, mesh-like vascular network formed initially through neovascularisation is highly ramified. Later, vascular network is normalised into a hemodynamically preferred tree-like structure. The normalisation process, termed vessel remodeling, leads to an organ-specific network architecture which better meets the metabolic needs of its surrounding tissue. As vessel growth and remodeling is found impaired in various disease states, several factors regulating vessel formation and branching morphology were identified over the past decades. However, while some of these factors have been undergoing clinical trials, their effects on transport properties of the altered vessel morphology are not fully elucidated yet. Establishing a perfusable human vasculature-on-a-chip (hVoC) model system, here we aim to investigate how vascular morphology correlates with flow field. Our hVoC model allows extensive quantitative analyses of network morphology and adaptive remodeling under fluid flow applied by a low-pressure syringe pump. Results of our analyses will contribute to the next generation therapeutics targeting vessel development.

DY 42.8 Thu 13:00 P1

Thermodynamics of active matter systems under coarse graining — •Robin Bebon and Thomas Speck — Institute for Theoretical Physics 4, University of Stuttgart, Heisenbergstraße 3, 70569 Stuttgart, Germany

Over the last decade, dynamic field theories have proven useful in the description of collective behavior and large-scale dynamics of active matter systems. However, despite their popularity, surprisingly little is known about how to capture thermodynamics on the level of such hydrodynamic descriptions. This is partially due to the fact that common approaches, based on symmetry arguments and conservation laws, typically neglect degrees of freedom that play a crucial role in quantifying the system's energetics, e.g., the self-propulsion mechanism. To advance, we propose a bottom-up approach that starts with a thermodynamically consistent microscopic model of catalytic particles driven by a constant affinity and derive effective hydrodynamic equations via explicit coarse graining. To ensure that information of the self-propulsion mechanism and its energy consumption is preserved on the macro-scale, we introduce an additional field, which for the considered model tracks the local rate of successful chemical events. We find that, near equilibrium, particle current and chemical field couple linearly through their respective thermodynamic forces, closely resembling linear irreversible thermodynamics. This provides an access point to investigate the thermodynamic properties of our field theory and compare the results with their microscopic counterparts.

DY 42.9 Thu 13:00 P1

The Liquid-Glass-Jamming Rheology of Soft Active Particles — •Roland Wiese[1], Klaus Kroy[1], and Demian Levis[2,3] — [1]Institute for Theoretical Physics, Leipzig University, 04103 Leipzig, Germany — [2]Departement de Fisica de la Materia Condensada, Facultat de Fisica, Universitat de Barcelona, Marti i Franquès 1, 08028 Barcelona, Spain — [3]University of Barcelona Institute of Complex Systems (UBICS), Facultat de Fisica, Universitat de Barcelona, Marti i Franquès 1, 08028 Barcelona, Spain

We study the linear and nonlinear rheology of an active Brownian particle suspension at different densities. In the low density and low shear limits the flow is Newtonian. In this regime its linear response viscosity can be calculated via the Green-Kubo autocorrelation method and is found to scale with an effective temperature. In the nonlinear regime of high shearing rates shear thinning is observed universally for all parameters considered in our study. Above the critical density of the glass transition the dynamics becomes arrested, marked by the appearance of a finite yield stress. Increasing the self-propulsion of the active particles shifts the glass transition to higher densities by melting the amorphous solid. The yield stress enables us to construct a phase diagram in the spirit of jamming phase diagrams, but exchanging temperature with activity. For suffienctly high activities glassy physics becomes suppressed and the yield stress scales with a power law in the density, known from jammed granular materials.

DY 42.10 Thu 13:00 P1

Wetting of reflecting plates by an Active Brownian fluid — •Matthieu Mangeat, Shauri Chakraborty, Adam Wysocki, and Heiko Rieger — Universität des Saarlandes, Saarbrücken, Germany

We study, using interacting active Brownian particles (ABP), the wall-wetting mechanism of active sedimenting fluid. We consider a minimal model of active particles under gravitational field, inside a two-dimensional rectangular box. An accumulation of particles near the bottom wall is observed, as well as the wetting of vertical plates by the rise of active particles against the gravity, even without any attractive force within the system. We characterize this wall-wetting by the meniscus height, calculated from stationary density profile and depending on the inter-particle repulsion. The maximum wetting height depends super-linearly on active sedimentation length for interacting ABP, and linearly for non-interacting ABP. We also observe two large vortices concentrated close to the meniscus, due to the persistence motion of ABP against the gravity. Moreover, with non-interacting ABP, a current flow is present near the boundaries for which we propose a coarse-grained description.

DY 42.11 Thu 13:00 P1

Force-free Ratcheting in Static Activity Landscapes — •Constantin Rein[1], Martin Kolář[2], Klaus Kroy[1], and Viktor Holubec[2] — [1]Leipzig University, Faculty of Physics and Earth Sciences, Institute for Theoretical Physics, Brüderstraße 16, 04081 Leipzig — [2]Charles University, Faculty of Mathematics and Physics, Department of Macromolecular Physics, V Holešovičkách 2, CZ-180 00 Praha

We study the possibility of rectifying active Brownian motion solely using time-independent activity landscapes. We argue that, in one dimension, spatially asymmetric activity does not suffice to induce directed transport, unless the activity is modulated in time or an additional potential is used, whereas, in higher dimensions, static activity landscapes alone can induce ratcheting. The underlying principle is similar to the ratcheting induced by asymmetric obstacles in microswimmer baths: swimmers with suitable orientations get channeled, while the others get trapped in low-activity regions until they lost their orientation. For landscapes with wedge-shaped low-activity regions, we numerically found an average transport velocity of the order of 1% of the particle's swim speed.

DY 42.12 Thu 13:00 P1

The nature of non-phononic excitations in disordered systems — •Walter Schirmacher[1,2], Matteo Paoluzzi[3], and Giancarlo Ruocco[2,4] — [1]Universität Mainz, Mainz, Germany — [2]Istituto Italiano di Tecnologia, Roma, Italy — [3]Universitat de Barcelona, Barcelona, Spain — [4]Universita di Roma "La Sapienza", Roma, Italy

We theoretically and numerically investigate the nature of the non-phononic excitations appearing in the vibrational spectrum of disordered materials of small systems, which do not allow for low-frequency waves (phonons). Using heterogeneous-elasticity theory and a new generalization, we are able to distinguish between two types of non-phononic vibrational excitations of disordered materials (glasses). A first type (Type-I) arises beyond the boson peak due to strong scattering from the structural disorder. These excitations are similar to the eigenvectors of random matrices. In very small systems, in the absence of low-frequency waves, the spectrum exhibits a gap, which, in a marginal-stable situation, may extend to zero frequency and features a DOS proportional to the square of the frequency. In such small systems, in a more stable situation, a second type of non-phononic excitations (Type-II) appears, which involve rotational oscillations around local frozen-in stresses. The frequency spectrum of these Type-II excitations is related to the interaction potential in the regime, where the potential contributions are small, rendering the frequency dependence non-universal. The frequently observed frequency scaling with the fourth power is shown to be an artifact due to the smooth tapering of the potential cutoff in the simulations.

DY 42.13 Thu 13:00 P1

Glass Transition in Modulated Liquids — •Abolfazl Ahmadirahmat[1], Michele Caraglio[1], Vincent Krakoviack[2], and Thomas Franosch[1] — [1]Institut für Theoretische Physik, Universität Innsbruck, Technikerstraße 21A, A-6020 Innsbruck, Austria — [2]Laboratoire de chimie, École normale supérieure de Lyon, 46 Allée d'Italie 69364 Lyon, Cedex 07, France

We have developed a theoretical description for the structural and dynamical properties of quasi-two-dimensional colloidal suspensions subject to periodic potentials using mode-coupling theory (MCT). We solve the MCT equations numerically for monodisperse hard disks modulated by a periodic external potential and, we show that the theory reduces to the conventional MCT equations of the glass transition for bulk systems if the external modulation vanishes. To do so, we elaborate numerical results for the long-time limits of suitably general-

ized intermediate scattering functions. We compare the nonergodicity parameter of a two-dimensional modulated liquid in zero modulation with the corresponding nonergodicity parameter for the bulk system in two dimensions.

DY 42.14 Thu 13:00 P1

Assembly of iron oxide nanocuboids directed by surface, ligand, and magnetic interactions — •Sindy J. Rodríguez Sotelo[1,2], Mario C.G. Paseggi Jr.[1,2], Carlos García[3], and Igor Stanković[4] — [1]Instituto de Física del Litoral IFIS-CONICET, Santa Fe, Argentina — [2]Facultad de Ingeniería Química, Universidad Nacional del Litoral UNL, Santa Fe, Argentina — [3]Departamento de Física and Centro Científico Tecnológico de Valparaíso-CCTVal, Universidad Técnica Federico Santa María, Valparaíso, Chile — [4]Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, Serbia

The direction of the dipole moment in the magnetite spherical nanoparticles is unrelated to the morphology particle. For non-spherical particles, a coupling between particle form and magnetic moment direction might result in unexpected behaviours, especially when the moment is not aligned along a particle symmetry axis [1,2]. We introduce energy models accounting for the directionality and magnitude of the van der Waals and dipolar interactions as a function of the shape of the nanocubes, illustrating the importance of the directional dipolar forces for the formation of the nanocube clusters, the dominance of the van der Waals multi-body interactions and exclusion forces of ligands. We illustrate how minimal energy structures depend on the assembly size, shape of the particles, and the balance of surface and magnetic dipolar coupling.

References [1] I. Stanković, *et al.* Nanoscale **12**, 19390, 2020. [2] L. Balcells *et al.* Nanoscale **11**, 14194, 2019.

DY 42.15 Thu 13:00 P1

Phase Behaviour of a Minimal Lattice Model with Chiral Interactions — •Boyi Wang[1,2], Patrick Pietzonka[1], and Frank Jülicher[1,3] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Institute of Physics, Chinese Academy of Sciences, Beijing, China — [3]Cluster of Excellence, Physics of Life, TU Dresden, Dresden, Germany

We introduce chiral interactions to a minimal lattice model based on the Ising model, adding second neighbour interactions that favour an L-shaped structure. We run Monte-Carlo simulations in equilibrium at low temperatures, and find two new ground states which exhibit chiral periodic tiling. We also study the phase behabiour analytically as a function of the strength of the chiral interaction and the external magnetic field. With number conservation, we observe the coexistence of chiral and achiral phases and the formation of droplets. Furthermore, we consider the role of chirality in this minimal lattice model with active driving forces.

DY 42.16 Thu 13:00 P1

Static and dynamical magnetic properties ferrofluid with ellipsoid-like nanoparticles — •Vladimir Zverev, Alla Dobroserdova, Ekaterina Ekaterina, Elena Pyanzina, and Alexey Ivanov — Ekaterinburg, Russia

A system of magnetic ellipsoids with a point dipole at the particle center is considered. We take into account different shape's anisotropy and different positions of the magnetic moment inside the particle (parallel and perpendicular to the main axis of the ellipsoid). In order to study this system, molecular dynamics simulations are used. The ratio of the main semi-axis to the additional one was used as a measure of the particle anisotropy. In particular, we have studied the system in which the particles have magnetic moments, but there is no dipole-dipole interaction between them. As a result, the initial magnetic susceptibility (magnetic characteristic) and the radial distribution function (structural characteristic) were calculated. For the initial susceptibility, the data obtained in computer simulations differ from the Langevin magnetization (theoretical ideal case) within the statistical error. The data for the Radial Distribution Function (RDF) also match within the calculation error. The next stage of research was to take into account dipole-dipole interparticle interactions and also will be presented.

DY 42.17 Thu 13:00 P1

Hopping conduction in networks with site energy disorder — •Quinn Emilia Fischer, Marco Bosi, and Philipp Maass — Fachbereich Physik, Universität Osnabrück, Barabarastraße 7, D-49076 Osnabrück, Germany

Understanding conductivities due to hopping motion in disordered systems is an important problem with various applications ranging from electron transport in amorphous semiconductors to ion transport in glasses [1,2]. A prominent model is that of particle hopping on a lattice with random site energies, where each lattice site can be occupied by at most one particle. For this model, a theory has been proposed, where transport properties are determined by a mapping onto a random resistor network [3]. By comparison with extensive kinetic Monte Carlo simulations for different types of site energy distributions, we show that this theory gives good predictions for small and high particle concentrations but is less accurate for intermediate concentrations. We present a refined theory which takes into account nearest neighbour correlations between occupation numbers in current carrying nonequilibrium steady states. This theory yields an improved prediction of conductivities and their activation energies in very good agreement with the Monte Carlo results.

[1] M. Bosi, P. Maass, J. Phys. Chem. C 125 6260 (2021).
[2] M. Bosi, P. Maass, Z. Phys. Chem. 236, 1055 2022).
[3] V. Ambegaokar, B. I. Halperin, J. S. Langer, Phys. Rev. B 4, 2612 (1971).