DY 29: Poster - Active Matter, Microswimmers and -fluidics, Statistical Physics Biosystems

Time: Tuesday 18:15–21:00   Location: Poster C

DY 29.1   Tue 18:15   Poster C
Stability and bifurcations in a model for active crystals
— ●Lukas Ophaus[1,2], Alexander Chervanyov[1,2], and Uwe
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The conserved Swift-Hohenberg equation [or Phase-Field-Crystal (PFC) model] provides a simple microscopic description of the thermodynamic transition from a fluid to a crystalline state [1,2]. The model can be combined with the Toner-Tu theory [3] for self-propelled particles to obtain a model for crystallization (swarm formation) in active systems [4]. Within the resulting active PFC model, resting and travelling crystals can be identified. The moving states migrate with a well-defined velocity while keeping their periodicity. These ordered swarms start to move at a critical value of an activity parameter.

We investigate the influence of this parameter on the linear stability of the homogeneous, fluid state. In addition, we use a one-dimensional version to explore the bifurcation structure at the onset of motion. Numerical continuation is applied to follow steady and travelling states to construct the bifurcation diagram.

[1] H. Emmerich, H. Löwen, R. Wittkowski, T. Gruhn, G. I. Tóth, G. Tegze and L. Gránásy, Adv. Phys. 61, 665 (2012)
[2] U. Thiele, A. J. Archer, M. J. Robbins, H. Gomez and E. Knobloch, Phys. Rev. E 87, 042915 (2013)
[3] J. Toner and Y. Tu, Phys. Rev. E 58, 4828 (1998)
[4] A. M. Menzel and H. Löwen, Phys. Rev. Lett. 110, 055702 (2013)

DY 29.2   Tue 18:15   Poster C
Large deviation statistics for self-propelled particles — ●Kevin Kleinbeck, Patrick Pietzonka, and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart

For a self-propelled particle, e.g., a Janus particle, we calculate the probability of fluctuations in the displacement during long time intervals. The particle is modeled with a translational and a rotational degree of freedom, with the latter affecting the direction of the constant self-propelling force. Moreover, we assume that the particle has a permanent magnetic moment that interacts with an external magnetic field. This symmetry breaking leads to a non-vanishing average velocity. We apply large deviation theory to calculate extreme fluctuations beyond the Gaussian regime.

For externally driven particles, the displacement along individual trajectories is proportional to the entropy production. As a central result of stochastic thermodynamics, the probability distribution of such an observable satisfies a fluctuation theorem relating the left and the right wing of the distribution. We show how the lack of the proportionality to entropy production for the displacement of self-driven particles affects the characteristic shape of the probability distribution. Moreover, we prove that the distribution satisfies a symmetry that is similar to the fluctuation theorem, but contains an additional term that depends only on the ratio between the field strength and the propulsion force.

DY 29.3   Tue 18:15   Poster C
Fluctuating Lattice Boltzmann simulations of microswimmers — ●Felix Winterhalter, Matthieu Marechal, and Klaus Mecke — Friedrich-Alexander-Universität, Erlangen, Germany

During the last years the interest in microswimmers has steadily increased. To gauge the effect of hydrodynamical interactions between the microswimmers and to include the flow of the solvent around the swimmer, a simulation technique with a good model for the solvent is required. Our method of choice is fluctuating Lattice Boltzmann simulations that includes thermal fluctuations, which are often important for synthetic swimmers. The currently existing particle simulation using the software WaLBerla is expanded to encompass self-propelled microswimmers to study their behavior in a variety of confining geometries and external fields. We are currently looking at ferromagnetic beads in an oscillating magnetic field and the flow field which is developing as a result of the collective motion.

DY 29.4   Tue 18:15   Poster C
Bead-spring microswimmers in a MPCD fluid — ●Hendrik

Ender and Jan Kierfeld — Theoretische Physik I, Technische Universität Dortmund, Germany

Bead-spring structures undergoing cyclic shape changes in a viscous liquid can serve as model systems for artifical microswimmers. Closed ring-like bead-spring models can propel by cyclic shape changes, for example, induced by cyclic expansion and contraction of springs.

Using multi-particle collision dynamics, we simulate different swimmer shapes and show that cyclic changes of linker lengths can give rise to a net swimming motion. The model can be generalized by including more beads and represents a step towards the simulation of bigger capsule-like swimmers, which propel by cyclic swelling and shrinking.

DY 29.5   Tue 18:15   Poster C
Turbulence driven clustering in nematic active particles — Devin Waas, ●Rebekka E. Breier, and Marco G. Mazza — MPI for Dynamics and Self-Organization, Göttingen

Many active swimmers are, especially in biological applications, exposed to a surrounding turbulent field. We assume the active particles to be self-propelled and to interact nematically with each other as well as with the turbulent field. We present a numerical study in terms of time-driven molecular dynamics simulations. The turbulent field is calculated via the so-called "Kraichnan model" which mimics the correct scaling behavior as given by the Kolmogorov law. We find that the turbulent field causes the active particles to cluster and investigate the clustering in detail. Moreover, the global alignment is destroyed by the turbulence.

DY 29.6   Tue 18:15   Poster C
The influence of intrinsic stochasticity on the stability and bifurcations of few-species networks — ●Johannes Falk and Barbara Drossel — TU Darmstadt, Germany

Intrinsic stochasticity in biological networks arises due to the limited number of individuals, which have stochastic birth and death rates. These individuals can be the biomolecules of gene regulation networks or the number of animals of an ecological population in foodwebs. Understanding the influence of stochasticity is important for assessing the stability of a system or for suppressing fluctuations in synthetic networks. Two important effects of intrinsic stochasticity are the shift of bifurcation points and of the eigenvalues of the stability matrix. Since explicit stochastic simulation is very time-consuming, analytical approaches for evaluating these effects were developed by various groups. We will apply these approaches to small reaction networks consisting of 2-4 nodes, which can be interpreted as foodweb modules or small chemical reaction networks.

DY 29.7   Tue 18:15   Poster C
The effect of small population sizes on the dynamics of biological networks with few nodes — ●Marc Mendler, Johannes Falk, and Barbara Drossel — Institut für Festkörperphysik, TU Darmstadt

Often, biological networks such as food webs or chemical reaction networks are described by deterministic coupled differential equations. However, in systems of only few individuals stochastic birth and death rates can modify the dynamics considerably, giving rise to macroscopic effects that cannot be explained by deterministic equations. When the intrinsic noise does not drive the system too far away from the deterministic limit, van Kampen's system-size expansion is a useful tool to calculate analytically the effects of stochasticity. Different groups have suggested different ways of applying the system-size expansion to small networks. We will compare these methods, determine their underlying assumptions and ranges of applicability, and compare analytical calculations to stochastic simulations.

DY 29.8   Tue 18:15   Poster C
Complex Polymers: DNA denaturation transitions — Yurij Holovatch[1,4] and ●Christian von Ferber[2,3,4] — [1]Institute for Condensed Matter Physics, NAS Ukraine, Lviv — [2]Applied Mathematics Research Centre, Coventry University, Coventry, UK — [3]Heinrich-Heine University, Dusseldorf — [4]Doctoral College, Statistical Physics of Complex Systems, Leipzig-Lorraine-Lviv-Coventry (L4)

We reconsider the Poland and Scheraga model for the DNA denaturation transition taking into account environmental effects. Here, we

apply field theoretical methods to discuss environmental effects on the nature of the transition. In particular we discuss variants of the transition that may occur due to particular properties of the environment. These are the presence of uncorrelated and power-law long-range correlated disorder which influence the transition as function of the power law exponent, the quality of the solution which may affect the self and mutual interaction of both single and double strands and combinations of these. We show that all of these have significant effects on the transition.

DY 29.9   Tue 18:15   Poster C

The evolution of network structure in an evolutionary food-web model without explicit population dynamics — •Tobias Rogge[1], Korinna T. Allhoff[2], and Barbara Drossel[1] — [1]TU Darmstadt, Germany — [2]UPMC Paris, France

Evolutionary foodweb models provide important insights into the stability and the functioning of ecosystems, since the network structure is a highly nontrivial outcome of the ongoing processes of species addition and species deletion. Here, we introduce and investigate an evolutionary food web model that includes no population dynamics but generates nevertheless a large variety of complex, multi-trophic networks. In this model, species are characterized by a few traits that are based on their body mass and that determine the connections to other species in the network. Starting from a simple initial network, the system evolves due to the addition of new species, which are modifications of existing species. Whether a new species can survive in the network depends on a criterion that takes into account the predators, the prey, and the competitors of the new species. When the new species survives, it changes the environment for other species, which will die out if they do not fulfil any longer the survival criterion.

Depending on the parameters, the long-term dynamics of the network can show layered structures, highly dynamical configurations with frequent extinctions, or frozen configurations that allow no mutant to survive. Using computer simulations and analytical calculations, we identify the conditions under which the different types of dynamical and structural patterns emerge.

DY 29.10   Tue 18:15   Poster C

Probing defects and correlations in the hydrogen-bond network of ab initio water — •Piero Gasparotto and Michele Ceriotti — Laboratory of Computational Science and Modeling, IMX, EPFL, 1015 Lausanne, Switzerland

Water is an unusual liquid and many of its unique properties are due to the presence of an highly-structured hydrogen-bond (HB) network that is populated by a wide variety of different coordination defects. Due to the structural constraints imposed by the HB network, coordination defects do not come alone, but clustered together. Here, we compute defect-resolved distribution functions from ab initio molecular dynamics to probe the radial and angular correlation between defects. In doing this, we shed light on how fluctuations from the ideal tetrahedral structure contribute to the total radial distribution function of liquid water. We also present a systematic comparison of the concentration of different defects and the structural correlations between them, with a variety of simulation protocols. For instance, we considered different temperature, system size, basis set, integrator timestep, cutoff for the plane waves, the modeling of van-der-Waals corrections, nuclear quantum effects or exact exchange. We also compare these results with those coming from empirical force field simulations. These comparisons show that regardless of the details of the choice of the water potential, the qualitative predictions of the defect distributions are very similar. The most significant effect can be attributed to dispersion interactions, that impact the most on the relative populations of the various defects.

DY 29.11   Tue 18:15   Poster C

Lateral migration of soft microparticles in wavy microchannels — •Matthias Laumann[1], Badr Kaoui[1], Georg Freund[1], Alexander Farutin[2], Chaouqi Misbah[2], Diego Kienle[1], and Walter Zimmermann[1] — [1]Theoretische Physik I, Universität Bayreuth, 95440 Bayreuth, Germany — [2]LiPhy, CNRS-Universite Joseph Fourier, F-28402 Saint-Martin d'Heres Cedex, France

We study the cross-streamline migration (CSM) of deformable particles in the limit of vanishing Reynold number in Poiseuille channel flow, which boundaries are spatially modulated. Using 1D dumbbells, 2D ring polymers, and 3D capsules, we demonstrate how the CSM can be modified when the waviness of the micro-channel is varied. Starting with the case of flat boundaries, these particles perform a CSM that is always directed towards the channel center. In the case of wavy boundaries, this centric motion may be reversed once the modulation amplitude exceeds a threshold, in which case the particles migrate off-center and approach a stationary trajectory, located between the walls and the channel center. The distance between such a trajectory and center can be increased by turning up the modulation amplitude, but depends also on other parameters such as the particle elasticity. The results shown are obtained via a perturbation calculation of the wavy Poiseuille flow in the limit of small modulation amplitudes, and is compared with those from Stokesian particle dynamics for arbitrary modulation amplitudes, showing good agreement. Out study suggests that the flow in wavy microfluidic channels may be exploited for the separation of particles.

DY 29.12   Tue 18:15   Poster C

Migration of soft particles in a modulated microchannel with flow along the grooves — •Winfried Schmidt, Matthias Laumann, and Walter Zimmermann — Theoretische Physik, Universitaet Bayreuth, Bayreuth, Germany

We find cross-streamline migration (CSM) of deformable particles in the low Reynold number limit in a plane Poiseuille flow with modulated boundaries and the flow along the grooves. CSM is studied for elastic 2D ring polymers, tetrahedrons and 3D capsules. We find two directions of cross-stream migration of particles. 3D particles migrate to the midplane between the two boundaries, similar as in the case of Poiseuille flow with plane boundaries [1]. In the case of modulated boundaries, the particles migrate in addition to the maxima and the minima of the distance between the two modulated boundaries. The migration velocity can be tuned by the amplitude of the boundary modulations. The migration velocity depends also on elasticity and size of the particles as well on the flow velocity. Our study suggests that the flow generated between wavy boundaries may be exploited for the separation of particles in modulated microfluidic channels.

[1] B. Kaoui, G. H. Ristow, I. Cantat, C. Misbah, W. Zimmermann, Phys. Rev. E 77 , 021903 (2008)

DY 29.13   Tue 18:15   Poster C

Phase-field model for phagocytosis — Kornelius Sücker[1], •Christian König[1], Walter Zimmermann[1], and Falko Ziebert[1,2] — [1]Theoretische Physik, Universität Bayreuth, Bayreuth, Germany — [2]Physikalisches Institut, Universität Freiburg, Freiburg, Germany

Phagocytosis is the process of engulfment of small (typically micron sized) particles by cells. It is used by unicellular organisms to take up nutrients, but also essential for the immune response in higher organisms. In contrast to the so-called endocytosis of nanoscale particles, which are taken up mainly by particle-induced membrane curvature, phagocytosis relies on active processes in the cytoskeleton. We here model the particle engulfment by a cell via a two-dimensional phase-field approach that allows to elegantly describe the moving cell boundary. The main mechanisms taken into account so far are the stimulation of actin polymerization and its associated propulsion force, as well as of motor contraction, by the presence of the particle.