

BP 35: Posters: Statistical Physics, Evolution, and Networks

Time: Thursday 17:15–20:00

Location: Poster B2

BP 35.1 Thu 17:15 Poster B2

Semiflexible polymers under the influence of a pressure driven Poiseuille flow — ●SEBASTIAN REDDIG and HOLGER STARK — Institut für Theoretische Physik, TU-Berlin

We introduce two different models for a semiflexible polymer under the influence of a pressure driven Poiseuille flow between two planar walls. In the first model we describe the polymer as a bead-spring model and use a discretized representation of the wormlike chain model for its bending elasticity. We neglect hydrodynamic interactions with the bounding walls but investigate the influence of the non-zero bead size which disturbs the external flow field. We explicitly calculate this disturbance from a series expansion following J.K.G. Dhont¹. It leads to additional terms in the equations of motion that cause cross-streamline migration in the Stokesian dynamics of the polymer. The direction of this migration can be controlled by varying the bead sizes. In the second model we approximate the beads by point particles and describe their hydrodynamic interactions with the two-wall Green tensor, derived by R.B. Jones², taking into account the no-slip condition at the bounding walls. Because the evaluation of the two-wall Green tensor consumes much computer time, we describe the polymer in this model by a simple dumbbell. Using Brownian dynamics simulations, we measure the center-of-mass probability density of the dumbbell and compare the results with theoretical predictions.

¹*An Introduction to Dynamics of Colloids*, Elsevier, (1996).

²*Spherical particle in Poiseuille flow between planar walls*, J. Chem. Phys., **121**, 483 (2004).

BP 35.2 Thu 17:15 Poster B2

Systematic Microcanonical Analyses of Polymer Adsorption Transitions — ●MONIKA MÖDDEL¹, WOLFHARD JANKE¹ und MICHAEL BACHMANN² — ¹Institut für Theoretische Physik, Universität Leipzig — ²Institut für Festkörperforschung, Theorie II, Forschungszentrum Jülich

Regarding the advances in processing and manipulating molecules at solid substrates, an understanding of the cooperative effects of finite chains is particularly desirable. We investigate this problem focusing on the adsorption transition [1,2] of a single chain near an attractive substrate. This is conveniently and to our knowledge for the first time done by a detailed microcanonical analysis [2] of densities of states obtained by extensive microcanonical Monte Carlo computer simulations. A remarkable consequence of the convexity of the microcanonical entropy is that for short chains and strong surface attraction the transition is accompanied by a decrease of the microcanonical temperature with increasing energy. Since this is a characteristic physical effect it might not be ignored in analyses of cooperative macrostate transitions in finite systems.

[1] M. Möddel, M. Bachmann, and W. Janke, J. Phys. Chem. B **113**, 3314 (2009).

[2] M. Möddel, M. Bachmann, and W. Janke, preprint.

BP 35.3 Thu 17:15 Poster B2

Spontaneous spiking in presence of delayed feedback — ●YUNYUN LI¹, GERHARD SCHMID¹, PETER HÄNGGI¹, and LUTZ SCHIMANSKY-GEIER² — ¹University of Augsburg, Augsburg, Germany — ²Humboldt-University Berlin, Berlin, Germany

Autapse is an interesting phenomena on neurons where axons synapsing on the same neuron's dendrites. This serves as delayed feedback mechanism in the dynamics of neuronal firing. Due the stochastic ion channel gating, there is intrinsic noise presented in the system which leads to spontaneous spiking[1]. Our modeling is done within a stochastic Hodgkin-Huxley model with self-delayed feedback of Pyragas-type. The delayed feedback introduced another time scale leading a competition between the delay time and characteristic intrinsic time of the Hodgkin-Huxley dynamics. Upon the intrinsic noise level and the coupling strength of the delayed coupling the firing exhibits bursting leading a multimodal structure in the interspike interval histogram. For the spontaneous spiking, both the mean interspike interval, and the coherence exhibits modulations upon varying the delay time.

[1] G. Schmid, I. Goychuk, P. Hänggi, Europhys. Lett. **56**, 22 (2001).

BP 35.4 Thu 17:15 Poster B2

Advection and Reaction in Open Flows — ●MITJA KLEIDER, IZ-

ABELLA BENCZIK, and JÜRGEN VOLLMER — Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen

Particles transported by blood flow can exhibit chaotic motion when wall irregularities are present [1]. This chaotic motion can influence physiological processes in the blood, for instance the activation and deposition of platelets that are involved in the thrombus formation.

To clarify the role played by chaotic advection in this process, we study a spatial model of a chaotic flow in which we define an activation and deposition region. Platelets can be deposited only if they are active when they enter the deposition region, i.e. if they have visited the activation region at a previous time. In this communication we discuss how chaoticity influences the deposition rate of platelets and enhances the growth of plaques and thrombi.

[1] Chaotic advection in blood flow, A. B. Schelin, Gy. Karolyi, A. P. S. de Moura, N. A. Booth, and C. Grebogi, Phys. Rev. E **80**, 016213 (2009)

BP 35.5 Thu 17:15 Poster B2

Finite-time thermodynamics and cyclic engines — ●DAVID ABREU and UDO SEIFERT — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

We study the finite-time thermodynamics of two simple systems and optimize the efficiency of a cyclic engine based on those two models. In the first case, the particle has two energy levels, one of which controlled by an external parameter ; in the second case, the particle is trapped in a harmonic potential whose position and stiffness are two externally controlled parameter. In both cases, we perform a measurement at the beginning and consider identical initial and final boundary conditions in energy. We show that optimization leads to discontinuous protocols. The second step consists in conceiving an optimal cyclic engine based on those two finite-time models. As opposed to the two-level model where the initial position is binary, the continuous model presents a different initial distribution at the beginning of each cycle, which leads to different solutions of the Fokker-Planck equation i.e. different optimal protocols. We emphasize the role of the measurement in the process and analyze the consequences of a feedback control during one cycle.

BP 35.6 Thu 17:15 Poster B2

Extended Fluctuation-Dissipation Theorem for Sheared Colloidal Suspensions — ●BORIS LANDER¹, THOMAS SPECK², and UDO SEIFERT¹ — ¹II. Institut für Theoretische Physik, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany — ²Department of Chemistry, University of California, Berkeley, CA 94720, USA

We consider suspensions of interacting colloidal particles driven by simple shear flow. For arbitrary strain rates, the recent extension of the fluctuation-dissipation theorem (FDT) to nonequilibrium steady states [1,2] enables us to study the response of single particles (tracer particles) perturbed by a small force. For particles interacting with a screened Coloumb potential, we obtain response and correlation functions through extensive numerical simulations for different densities and strain rates. For higher densities these curves show oscillations, which are explained qualitatively. The time-integrated version of the extended FDT connects the single particle mobility with the diffusion coefficient through an integrated excess function. In addition, we analyze features of this system analytically in the simple model of a single particle in a harmonic potential driven by shear flow.

[1] T. Speck and U. Seifert, Europhys. Lett. **74**, 391, (2006)

[2] T. Speck and U. Seifert, Phys. Rev. E **79**, 040102(R), (2009)

BP 35.7 Thu 17:15 Poster B2

Effect of thermostating and electrostatics on the solution structure and dynamics of signal transduction of the wildtype-LOV1 domain of phototropin — EMANUEL PETER, BERNHARD DICK, and ●STEPHAN BAEURLE — Institut für Physikalische und Theoretische Chemie, Universität Regensburg, Universitätsstr. 31, 93053 Regensburg, Deutschland

Phototropins are photoactive proteins in plants and algae, which consist of 2 LOV-(light oxygen voltage sensitive)-domains and 1 kinase domain. Each LOV-domain contains a noncovalently bound flavin-mononucleotid-(FMN)-chromophor, which after absorption of blue

light at around 450 nm undergoes a photoreaction with a cysteine-residue attached to an apoprotein, inducing a signal in the organism via the kinase-domain. Both the signal transduction as well as the mechanism of the photoreaction of these domains are still only poorly understood. In this presentation we show results of molecular dynamics simulations, where we investigated the effect of thermostating and long-range electrostatics on the solution structure and dynamics of signal transduction of the wildtype LOV1-domain of the green algae *Chlamydomonas reinhardtii*. By comparing our calculation results with recent simulation and experimental data, we demonstrate that these issues have an important influence on the equilibrium structure and the time-evolution of the system.

BP 35.8 Thu 17:15 Poster B2

Thermodynamics of polymers anchored to fluctuating tethered membranes — ●STEFFEN KARALUS^{1,2}, WOLFHARD JANKE¹, and MICHAEL BACHMANN² — ¹Institut für Theoretische Physik, Universität Leipzig, Germany — ²Soft Matter Systems Research Group, Institut für Festkörperforschung (IFF-2), Forschungszentrum Jülich, Germany

By means of extensive Monte Carlo simulations we study a coarse-grained model for a bead-and-spring polymer anchored to a two-dimensional tethered (polymerized) membrane embedded into three-dimensional space [1]. Our model includes interactions within the polymer and the membrane as well as an attractive polymer-membrane potential. In order to identify structural transitions, we investigate fluctuations of thermodynamic quantities in dependence of the polymer-membrane interaction strength. Applied methods include generalized ensemble methods such as multicanonical simulations and parallel tempering.

[1] H. Popova and A. Milchev, *J. Chem. Phys.* **127**, 194903 (2007); *J. Chem. Phys.* **129**, 215103 (2008)

BP 35.9 Thu 17:15 Poster B2

Role of hydrodynamic anisotropy for protein-protein encounter — ●JAKOB SCHLUTTIG, CHRISTIAN KORN, and ULRICH SCHWARZ — Institut für Theoretische Physik, Universität Heidelberg, 69120 Deutschland

Protein-protein interactions in cells comprise both transport and reaction steps. Although both single proteins and intermediate complexes are usually not spherical, the role of anisotropy for protein-protein encounter has not been systematically studied before. Using a Langevin equation approach, we quantify the influence of anisotropy on the encounter rate of model particles. We consider a purely geometric definition of the encounter complex by introducing spherical encounter patches located on the surface of ellipsoidal particles. We investigate the encounter rate k at various aspect ratios ξ for different locations of the encounter patches and different concentrations. We show that the dependence of k on ξ can be mainly attributed to steric effects while the altered diffusion behaviour has a rather small effect. In general one expects that rotational diffusion crosses over to isotropic behaviour for sufficiently long times. We analytically calculate the three-dimensional crossover time and show that it is much smaller than typical protein encounter times, in good agreement with our simulation results.

BP 35.10 Thu 17:15 Poster B2

Die zelluläre Proteinsynthese, ein kosmisches Fraktal der E8-Grp. — ●NORBERT SADLER — 85540 Haar ; Wasserburger Str. 25a

Die Struktur des expandierenden Universums kann mit der E8-Gruppe abgebr. definiert werden: $E8 = 1/(5/9 \cdot H) = 8,56 \cdot 10^{17}$ mit $H = 64,7 \text{ km/mpcs}$. Die E8-Symmetriegruppe kann als ein synth. kosm. Ribosom verstanden werden, dass unter Wechselwirkung mit der beschl. kosmischen Expansion H , in einer fraktalen Selbstorganisation, $E8/c = 2,86 \cdot 10^9$ Basen-Paare translatiert. Das kosm. E8-Analogon zur zellulären Umsetzung der Erbinformation ist ein synth. Ribosom, $(4 \text{ Basen} \cdot 1 \text{ Tripl}) = 64$ Wörter, durch die die 20 Aminosäuren, unter Einwirkung der kosm. Expansion, gefädelt, transkribiert und synthetisiert werden. Die algebraisch-kosm. Darstellung der E8-Translation: $E8/c = (H = 64,7 \text{ km/mpcs}) \cdot (4 \text{ Bas} \cdot 1 \text{ Tripl}) \cdot (4/3 \text{ Prot}) \cdot (2 \cdot 19 \text{ Aminos.})$

Algebra E8: $64,7 \cdot 64 \cdot 4/3 \cdot 2 \cdot 19 = 2,86 \cdot 10^9$ Basen-Paare

Die abgebr. Darstellung über die 32 Kristall-Klassen:

$E8/c = (\alpha(QCD)/\alpha(QED)) \cdot (32 \text{ Kr. Kl.}) \cdot (4 \cdot 3) \cdot (2 \cdot 19 \text{ Aminos.})$

Algebra E8: $8/3 \cdot 32 \cdot 64 \cdot 2 \cdot 19 = 2,86 \cdot 10^9$ Basen-Paare. Die Menge der über E8 translatierten Basen-Paare entspricht in etwa der des Human-Genoms. Erkenntnis: Das expandierende Universum ist in der E8-Darstellung ein kosmisches Organell

BP 35.11 Thu 17:15 Poster B2

The influence of spatial correlations and fractal properties of bacterial patterns on colony extinction — ●FLORENTINE MAYER and ERWIN FREY — Arnold Sommerfeld Center for Theoretical Physics (ASC) and Center for NanoScience (CeNS), Ludwig-Maximilians-Universität München, Theresienstrasse 37, D-80333 München, Germany

Bacterial communities represent complex and dynamic ecological systems. They appear in the form of free-floating bacteria as well as biofilms in nearly all parts of our environment. They are highly relevant for human health and disease. Spatial patterns arise from heterogeneities of the underlying landscape or are self-organized by the bacterial interactions, and play an important role in maintaining species diversity. We investigate mechanisms for extinction of the population with our automaton model for a bacterial biofilm in fluctuating environments, where each bacterium can take two different phenotypes, whose growth and death rates depend on the environmental conditions. Employing stochastic simulations we find that the typical time until extinction occurs depends on the system size. We study the maximum of cluster mass over time during an extinction process. Furthermore the fractal properties of the patterns that existed before the extinction are characterized in regard to their influence on the extinction behaviour.

BP 35.12 Thu 17:15 Poster B2

Fixation time in zero-sum and non zero-sum cyclic coevolution — ●MARKUS SCHÜTT and JENS CHRISTIAN CLAUSSEN — Inst. für Neuro- und Bioinformatik, Universität zu Lübeck

In the territorial and mating behavior of *Uta stansburiana*, as well as in the colicin secretion and resistance, cyclic coevolutionary dynamics is observed. The coevolutionary payoff matrix has the structure of the rock-paper-scissors (RPS) game, which typically is zero-sum: what one player loses, equals the gain of the winning opponent. In biology, payoffs are difficult to measure, but in general the game can deviate from the zero-sum condition, and the examples mentioned above represent the positive and negative sum cases. In previous work, we have shown that a positive-sum game can stabilize the coexistence (and therefore preserve biodiversity) for a population size below a critical value [1], similar as for the Moran process in cyclic bimatrix games [2]. Here [3], we investigate the scaling of the fixation time and show that the crossover from polynomial to exponential scaling is consistent with the drift reversal as demonstrated in [1].

[1] JC Claussen and A Traulsen, *Phys. Rev. Lett* (2008)

[2] JC Claussen, *Eur. Phys. J.* (2007)

[3] M Schütt and JC Claussen (in preparation)

BP 35.13 Thu 17:15 Poster B2

Investigating the chemo-mechanical properties of two-dimensional actin networks — KAI UHRIG^{1,2}, RAINER KURRE^{1,2}, ●MARTIN STREICHFUSS^{1,2}, FRIEDRICH ERBS^{1,2}, SIMON SCHULZ^{1,2}, ANABEL CLEMEN^{1,2}, TAMAS HARASZTI^{1,2}, CHRISTIAN BÖHM^{1,2} und JOACHIM SPATZ^{1,2} — ¹MPI for Metals Research, Dept. Spatz, Heisenbergstr. 3, 70569 Stuttgart — ²Univ. of Heidelberg, Biophys. Chem. Dept., INF 253, 69120 Heidelberg

The actin cortex, a quasi two-dimensional network of actin, plays an important role in cell stability, motility and viscoelasticity. In vivo, its characteristic properties are controlled by various crosslinkers, such as actin binding proteins or ions. To investigate the influence of a specific crosslinker on the network's behaviour exclusively we create and probe biomimetic models of the actin cortex. This is realized using microbeads trapped by holographic optical tweezers (HOTs) as scaffold for the actin filaments. With this technique we are able to create actin networks in arbitrary geometry and determine the forces exerted by different crosslinkers. Using a special microfluidic flowcell we have full control over the chemical environment in our experiments. The acting forces are measured by highspeed imaging, whereas simultaneous fluorescence microscopy yields information about the structure and density of the actin network. In another approach we use micro-pillars as framework and measure unzipping forces of crosslinked actin filaments.

BP 35.14 Thu 17:15 Poster B2

Coexistence and phenology of mass-selective predators — ●LAURIN LENGERT, BARBARA DROSSEL, and CHRISTIAN GUILL — TU Darmstadt, Hessen, Deutschland

We study the phenology of predator species, i.e. the chronological

succession of species that consume the same prey species within a year. Phenology is modeled by using body-mass dependent attack rates. While prey individuals that are very small compared to predators can easily hide from predators, larger prey individuals have a higher chance to directly escape attacks. This leads to an unimodal capture rate as function of predator and prey size with a maximum at intermediate predator-prey body-mass ratios.

We model the prey to grow during the observed period while the larger predators have a constant body mass (assuming that new born predator individuals are hatching and growing during a different period of the year). Differently sized predator species thus differ in the time when their attack rates on the prey species are maximal.

We analyze the effect of predator phenology on the system's capability to support several predator species with different mean individual body masses and present results concerning minimal size differences between coexisting predators as well as potential invasion scenarios.

BP 35.15 Thu 17:15 Poster B2

The effect of body mass and adaptive foraging on food web robustness — ●LOTTA HECKMANN, CHRISTIAN GUILL, and BARBARA

DROSSEL — Institut für Festkörperphysik, TU Darmstadt

Revealing the mechanisms promoting the stability of complex food webs remains a challenge for theoretical ecologists. One apparently stabilizing factor identified recently is the incorporation of allometric scaling, i.e., the influence of the body mass of a species on its metabolic rate, into the differential equations of population dynamics. By this, predator-prey interaction rates become body-mass dependent. Another mechanism contributing to the stability of food webs is adaptive foraging, that is, the capability of predators to focus on more profitable prey.

We numerically investigated the impact of the combined effects of allometric scaling and adaptive foraging on the robustness of food webs, considering different time scales of adaptation (evolutionary vs. behavioural changes) and different predator-prey body mass ratios. Our simulations include nonlinear population dynamics equations with Holling type II functional responses and intraspecific competition. The simulations were performed for different stochastic network structures, such as random graphs or the niche model. Additionally, we analyze in more detail the mechanisms by which adaptive foraging stabilizes food webs by using modules of a small number of interacting species.