CPP 29: Biopolymers and Biomaterials III (jointly with BP)

Time: Wednesday 15:00–17:45 Location: ZEU 260

CPP 29.1 Wed 15:00 ZEU 260

Spontaneous Flows of Active Polar Gels between two Rotating Cylinders — Marc Neef[1], Sebastian Fürthauer[2], •Stephan Grill[2], Frank Jülicher[3], and Karsten Kruse[1] — [1]Theoretische Physik, Universität des Saarlandes, 66041 Saarbrücken — [2]Max Planck Institute of Molecular Cell Biology and Genetics, 01307 Dresden — [3]Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden

Active Biological matter, e.g. cell tissues or the cytoskeleton can flow spontaneously. In situations, where the material is confined, the flow pattern depends on the geometry of the domain and the boundary conditions, as well as on the system's active properties. We investigate the influence of these factors by theoretically analyzing the equations of motion for active polar fluids in the space between two coaxial cylinders that rotate at a given frequency. In striking contrast to the behavior of uniform flows in open geometries, we find that in the confined case, activity can also stabilize uniform flow patterns.

CPP 29.2 Wed 15:15 ZEU 260

Brownian motion of stiff filaments in confined media — •Nikta Fakhri[1,4], Fred MacKintosh[2], Brahim Lounis[3], Laurent Cognet[3], and Matteo Pasquali[4] — [1]Fakultät für Physik, III. Physikalisches Institut - Biophysik , Georg-August-Universität, Göttingen, Germany — [2]Department of Physics and Astronomy, Vrije Universiteit, Amsterdam, The Netherlands — [3]Centre de Physique Moléculaire Optique et Hertzienne, Université Bordeaux, and CNRS, Talence, France — [4]Department of Chemical and Biomolecular Engineering, The Smalley Institute for Nanoscale Science and Technology, Rice University, Houston, Texas, USA

The thermal motion of stiff filaments in a crowded environment underlies the behavior of such disparate systems as polymer materials, nanocomposites, and the cell cytoskeleton. Despite decades of theoretical study, the fundamental dynamics of such systems remains a mystery. Using near-infrared video microscopy, we study the thermal diffusion of individual single-walled carbon nanotubes (SWNTs) confined in porous agarose networks. Surprisingly, we find that even a small bending flexibility strongly enhances their motion: the rotational diffusion constant is proportional to the filament bending compliance and is independent of the network porosity. This study establishes definitively the reptation dynamics of stiff filaments and provides a framework to tailor the mobility of SWNTs in confined environments.

CPP 29.3 Wed 15:30 ZEU 260

Depletion forces between single actin filaments — Martin Streichfuss[1,2], •Tamas Haraszti[1,2], and Joachim P. Spatz[1,2] — [1]Max-Planck Institute for Metals Reseach, Stuttgart, Germany — [2]Biophysical Chemistry, University of Heidelberg, Heidelberg, Germany

Filamentous actin is one of the most investigated components of the cytoskeleton in cells. The polymerization process forming the filaments from their globular actin subunits is well known to play a crucial role in cell protrusion, such as the formation of filopodia and lamellopodia.

Recent theoretical predictions suggested that the process of bundle formation of the newly polymerized actin filaments may also contribute to the forces pushing the cell membrane ahead in such protrusions. Rheology experiments reported during the last two decades on in-vitro actin gels have provided indirect information on the interactions with or without various crosslinker agents present.

We have measured the forces acting between two actin filaments using holographic optical tweezers during the bundling process in the presence of divalent cations (Mg^{2+}, 25-200 mM) or polyethylene glycol (PEG) polymer as depletion agents. The results indicate forces up to about 0.1 - 0.2 pN in a saturation manner, independent of the concentration of the magnesium ions above 50 mM.

The magnitude of these forces is comparable to the forces produced by the polymerization ratchet, providing a direct hint that the bundling forces may contribute to the formation of cellular protrusions significantly.

CPP 29.4 Wed 15:45 ZEU 260

Coarse Grained Simulations of Biopolymers: Effects of Finite Damping and Hydrodynamic Interactions — Uwe Winter and •Tihamer Geyer — Center for Bioinformatics, Saarland University, Saarbrücken

In the coarse grained Brownian Dynamics simulation method the many solvent molecules are replaced by random thermal kicks and an effective friction acting on the particles of interest. For Brownian Dynamics the friction has to be so strong that the particles' velocities are damped much faster than the duration of an integration timestep. Here we show that this conceptual limit can be dropped with an analytic integration of the equations of damped motion. In the resulting Langevin integration scheme our recently proposed approximate form of the hydrodynamic interactions between the particles [1] can be incorparated conveniently, leading to a fast multi-particle propagation scheme, which captures more of the short-time and short-range solvent effects than standard BD. Comparing the dynamics of a bead-spring model of a short peptide, we recommend to run simulations of biological molecules and polymers with the Langevin type finite damping and to include the hydrodynamic interactions [2].

[1] Geyer, Winter, *J. Chem. Phys.* **130** (2009) 114905
[2] Winter, Geyer, *J. Chem. Phys.* **131** (2009) 104102

CPP 29.5 Wed 16:00 ZEU 260

Transport of a semiflexible filament in a network — •Teresa Bauer[1], Felix Höfling[2], Erwin Frey[1], and Thomas Franosch[3] — [1]Arnold Sommerfeld Center (ASC) for Theoretical Physics and Center for NanoScience (CeNS), Fakultät für Physik, Ludwig-Maximilians-Universität München, Germany — [2]Max-Planck-Institut für Metallforschung, Stuttgart and Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Germany — [3]Institut für Theoretische Physik, Universität Erlangen-Nürnberg, Germany

The cytoskeleton of a cell is comprised of a network of various biopolymers. A prominent example is the filamentous actin, a semiflexible polymer studied extensively also in vitro. The transport of a single semiflexible filament in a strongly entangled network is highly directed along the confining tube formed by the surrounding network.

We have investigated the dynamics of a semiflexible filament in a plane in the presence of immobilized obstacles mimicking the constraints of the crosslinked network. The inextensibility constraints are encoded via a bead-rod-algorithm extended by a suitable collision rule and extensive simulations are performed. In particular we quantify the translational and rotational diffusion investigated for a broad density range and visualize the dynamics using representative animations. Furthermore we discuss issues of numerical stability.

15 min. break

CPP 29.6 Wed 16:30 ZEU 260

Interplay of conformational degrees of freedom and crosslink binding in filamentous biopolymer bundles — •Claus Heussinger — Institute for Theoretical Physics, University of Goettingen, Germany

Crosslinked F-Actin bundles constitute principal components of a multitude of cytoskeletal processes and play key roles in many cellular functions. Much of the special properties of crosslinked biopolymer bundles derives from the interplay of bundle conformational degrees of freedom with the internal binding status of the crosslinking agent. Depending on probing time- and length-scales this interplay can lead to interesting dynamical effects as well as non-trivial elasto-plastic phase-behavior. By employing theoretical considerations combined with Monte-Carlo simulations, we will discuss some aspects of the internal dynamics of the cross-linker whose binding affinity serves to stabilize the bundle. We show how an imposed bundle deformation modifies the equilibrium binding constant and even allows for the coexistence of different bundle states.

CPP 29.7 Wed 16:45 ZEU 260

Interfacial effects on amyloid fibrilization — •Chiu Fan Lee[1], Létitia Jean[2], Chongsoo Lee[2], Michael Shaw[2], and David J. Vaux[2] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Sir William Dunn School of Pathology, Oxford, UK

Amyloid accumulation is associated with pathological conditions, including type II diabetes and Alzheimer's disease. Lipids influence amy-

loidogenesis and are themselves targets for amyloid-mediated cell membrane disruption. Amyloid precursors are surface active, accumulating at hydrophobic-hydrophilic interfaces (e.g., air-water), where their biophysical and kinetic behaviors differ from those in the bulk solution with significant and underappreciated consequences. Using a combined experimental and theoretical approach, we demonstrate amyloid fibrilization is critically dependent on the presence of air-water interface (AWI). Furthermore, we showed that the role of membranes in amyloidogenesis has been previously underestimated; in an *in vivo*-like situation (with no AWI), anionic liposomes (containing dioleoylphosphatidylglycerol) enhanced islet amyloid polypeptide (IAPP) fibrilogenesis far more than described previously in conventional assay conditions (in the presence of an AWI). These findings have implications for the protein misfolding field and in assay design to target toxic protein aggregation.

Reference: L. Jean, C. F. Lee, C. Lee, M. Shaw, D. J. Vaux. FASEB J. **24**, 309 (2010).

CPP 29.8 Wed 17:00 ZEU 260

Keratin homogeneity in the tail feathers of peacocks — •Silvia Pabisch[1,2], Stephan Puchegger[1], Ingrid M. Weiss[3], Helmut O. Kirchner[3], and Herwig Peterlik[1] — [1]University of Vienna, Faculty of Physics, Vienna, Austria — [2]Vienna University of Technology, Institute for Materials Chemistry, Vienna, Austria — [3]INM-Leibniz Institute for New Materials, Saarbrücken, Germany

X-ray diffraction studies successfully clarified the structure of avian feathers: Each filament has a helical structure with four repeating units per turn.[1] The structure of avian feathers is very stable though their relative density is low. The keratin structure in the cortex of peacocks' feathers is studied by X-ray diffraction along the feather, from the calamus to the tip. It changes considerably over the first 5 cm close to the calamus and remains constant for about 1 m along the length of the feather. We attribute the X-ray patterns to a shrinkage of a cylindrical arrangement of beta-sheets, which is not fully formed initially. In the final structure, the crystalline beta-cores are fixed by the rest of the keratin molecule. The hydrophobic residues of the beta core are locked into a zip-like arrangement. Tensile and compression tests are additionally performed in-situ to follow the structural change as consequence of varying load.

[1] R.D.B. Fraser and D.A.D. Perry, J. Struct. Biol. 162 (2008) 1-13.

CPP 29.9 Wed 17:15 ZEU 260

Thermophoresis quantifies the Conformation and Stability of Biomolecules — •Christoph Jens Wienken, Philipp Baaske, Stefan Duhr, and Dieter Braun — Systems Biophysics, LMU München, Germany

Stability and conformation of biomolecules is important in the field of biology, medical diagnostics and biotechnology. We developed a method which measures both parameters using Microscale Thermophoresis, an all-optical technique which only uses 250nl of sample. Thermophoresis is the directed movement of molecules in a temperature gradient. It depends on surface characteristics of the molecule, such as size, charge and hydrophobicity [1]. Its sensitivity for small changes in above parameters was recently shown by analyzing the binding reactions of DNA aptamers and a variety of proteins [2,3].

When measuring thermophoresis over temperature, information about the thermal stability of biomolecules are accessible. We find clear melting transitions and resolve intermediate conformational states. With this it is possible to analyze single nucleotide polymorphisms, DNA modifications and conformational states. The thermophoretic melting analysis is also applicable to proteins where unfolding patterns comparable to scanning calorimetry are found.

[1] Duhr,S & Braun,D Proc. Natl Acad. Sci. USA 103, 19678 (2006).
[2] Baaske,P et al. Angew. Chem. Int. Ed. 49, 2238 (2010).
[3] Wienken,CJ et al. Nat. Commun. 1:100 (2010).

CPP 29.10 Wed 17:30 ZEU 260

Liquid-liquid phase separation in protein solutions induced by multivalent counter ions — •Marcell Wolf, Fajun Zhang, Felix Roosen-Runge, Andrea Sauter, and Frank Schreiber — Institut für Angewandte Physik, Auf der Morgenstelle 10, Universität Tübingen, 72076 Tübingen, Germany

The liquid-liquid phase separation (LLPS) in concentrated protein solutions plays an important role for protein crystallization as well as protein-association related diseases, such as the sickle cell anemia and eye cataracts, etc [1]. Here, we show that the LLPS can be induced in protein solutions by using a multivalent salt like Yttrium Chloride (YCl_3). The phase diagram of proteins with YCl_3 in the c_p (protein concentration) - c_s (salt concentration) plane is determined. The protein solution undergoes a phase-separation upon adding salt up to a critical value c*. Further increasing c_s to c** the precipitates dissolve and the system turns back to a homogenous solution. This is a reentrant phase behavior [2]. In the condensed regime between c* and c** the system is thermodynamically equivalent to the phase behavior of a hard sphere with short range interactions, which exhibits a stable gas-solid transition and a metastable LLPS. The phase boundary is determined by UV and X-ray absorption. The effective protein-protein interactions in solutions upon LLPS are investigated by SLS and SAXS. The resulting interaction potential has been compared and discussed based on the thermodynamic criteria. [1] J.D. Gunton, A. Shiryayev, D. L. Pagan, Protein Condensation, 2007, Cambridge University Press, [2] F. Zhang et al., Phys. Rev. Lett. 101 (2008) 148101