

## BP 6: Biopolymer Conformation and Dynamics

Time: Monday 14:30–16:00

Location: H44

BP 6.1 Mon 14:30 H44

**Semiflexible polymers: Dependence on ensemble and boundary orientations** — ●DEBASISH CHAUDHURI — MPIPKS Dresden, Noethnitzer Str. 38, 01187 Dresden

We show that the mechanical properties of a worm-like-chain (WLC) polymer, of contour length  $L$  and persistence length  $\lambda$  such that  $t = L/\lambda \sim \mathcal{O}(1)$ , depend both on the ensemble and the constraint on end-orientations. In the Helmholtz ensemble, multiple minima in the free energy near  $t = 4$  persists for all kinds of orientational boundary conditions. The qualitative features of projected probability distribution of end to end vector depend crucially on the embedding dimensions. A mapping of the WLC model, to a quantum particle moving on the surface of an unit sphere, is used to obtain the statistical and mechanical properties of the polymer under various boundary conditions and ensembles. The results show excellent agreement with Monte-Carlo simulations.

BP 6.2 Mon 14:45 H44

**DNA: From rigid base-pairs to semiflexible polymers** — ●NILS BECKER<sup>1</sup> and RALF EVERAERS<sup>1,2</sup> — <sup>1</sup>Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden — <sup>2</sup>Laboratoire de Physique, ENS Lyon, 46, allée d'Italie, 69364 Lyon, France

The sequence-dependent elasticity of double-helical DNA on a nm length scale is captured by the rigid base-pair model, whose strains are the relative position and orientation of adjacent base-pairs. Corresponding elastic potentials have been obtained from all-atom MD simulation and from high-resolution structural data. On the scale of a hundred nm, DNA is successfully described by a continuous worm-like chain model with homogeneous elastic properties. These are characterized by a set of four elastic constants [1], recently measured on single molecules [2,3].

We present a theory that links these experiments on different scales by systematic coarse-graining. We find that the average elastic constants for random sequence DNA show reasonable agreement. However for short chains, the variability of structure and stiffness with sequence leads to large deviations from the average, including non-Gaussian bend angle distributions and elevated looping probabilities.

[1] J. F. Marko and E. D. Siggia, *Biophys J* 73, 2173, 1997[2] T. Lionnet et al., *Phys Rev Lett* 96, 178102, 2006[3] J. Gore et al., *Nature* 442, 836, 2006

BP 6.3 Mon 15:00 H44

**Force-induced structural transitions in cross-linked DNA films** — ●ALEXANDER ANDRÉ<sup>1,2</sup>, THEO FISCHER<sup>1</sup>, GEORG MARET<sup>1</sup>, and THOMAS GISLER<sup>1</sup> — <sup>1</sup>Universität Konstanz, Konstanz, Germany — <sup>2</sup>Université Louis Pasteur, Strasbourg, France

Single-molecule experiments have revealed that double-stranded DNA can be extended by about 60% beyond its natural contour length at nearly constant force [1,2]. The origin of this plateau in the force-extension curve is however still under debate, mainly since no direct structural information has so far been obtained from single overstretched DNA molecules. We propose an experimental approach to investigating the structure of overstretched DNA, using oriented DNA films obtained by wet-spinning. Randomly cross-linking DNA by intercalation compounds and covalent bonds between nucleobases results in elastomeric films which can be reversibly overstretched. We characterize the structure of these cross-linked films under mechanical load with X-ray diffraction and birefringence experiments.

[1] P. Cluzel, A. Lebrun, C. Heller et al., "DNA: An Extensible Molecule," *Science* 271, 792-794 (1996). [2] S. B. Smith, Y. Cui, A. C. Hausrath et al., "Stretching DNA beyond its B-form contour length," *Biophys. J.* 68, A250 (1995).

BP 6.4 Mon 15:15 H44

**Fluctuating polymer rings** — ●KAREN WINKLER and ERWIN FREY — Arnold Sommerfeld Center for Theoretical Physics and CeNS,

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Geometric constraints have been proven to induce interesting behavior on polymers. We consider polymer bundles confined to a ring-like structure. This constraint causes an additional bending stiffness and coupling of bending and twisting modes. To describe polymer bundles we derived an analytic model for a semiflexible polymer ring with anisotropic bending stiffness and twist stiffness. This model predicts the mean square diameter of a ribbonlike ring thus giving a novel parameter to determine bending and twist stiffnesses of polymer bundles in experiments.

Furthermore the asymmetric shape of polymer rings with symmetric cross section is investigated over the whole range of flexibility by Monte Carlo simulations. For semiflexible polymers a scaling argument explains the change of the polymer's asphericity with increasing flexibility.

BP 6.5 Mon 15:30 H44

**Conformation control of plasmid DNA on a solid substrate** — ●WEI ZHUANG, HUA LIANG, NIKOLAI SEVERIN, and JÜRGEN P. RABE — Institut für Physik, Humboldt University Berlin, Berlin, Germany

The conformation of single DNA molecules may be controlled by stretching them with optical tweezers [1] or a scanning force microscope (SFM) probe [2]. In recent work it has been demonstrated that a highly oriented pyrolytic graphite (HOPG) surface coated by self-assembled alkylamine amphiphiles can serve as a substrate on which single DNA molecules can be manipulated by an SFM probe [3]. A disadvantage of the above mentioned techniques is that they have to be applied to one molecule at a time. Here we describe a preparation of an amphiphile coated HOPG surface, on which the conformation of plasmid DNA can be fully controlled across the whole surface. By varying the concentration of amphiphiles on the surface, plasmid DNA molecules exhibit different conformations ranging from supercoiling, relaxed open circle, to overstretching. Particularly, when DNA molecules are adsorbed on 60% amphiphile sub-monolayer covered HOPG, upon mild annealing the DNA molecules can be overstretched up to 1.5 times of their B-form length due to steric repulsion between adjacent alkyl chains. It is suggested that a fully screened amphiphile-DNA complex is formed on the surface. The spontaneous overstretching of many DNA molecules at a time may become useful for the development of a fast processing genomic analysis chip. 1. S.B.Smith, et. al *Science* 271 (1996) 795 2. M.Rief, et. al *Nat. Struct. Biol.* 6 (1999) 346 3. N.Severin, et. al *Nano Lett.* 4 (2004) 577

BP 6.6 Mon 15:45 H44

**How does a straight polymer relax?** — ●BENEDIKT OBERMAYER<sup>1</sup>, OSKAR HALLATSCHKE<sup>2</sup>, ERWIN FREY<sup>1</sup>, and KLAUS KROY<sup>3</sup> — <sup>1</sup>ASC und CeNS, LMU München — <sup>2</sup>Lyman Laboratory of Physics, Harvard University — <sup>3</sup>ITP, Universität Leipzig

Although the relaxation dynamics of semiflexible polymers from an initially straight conformation has been discussed extensively in the literature, this seemingly simple problem involves nontrivial physics that is not yet completely understood. This is partly due to the ambiguous meaning of "initially straight", for which various realizations are conceivable. The filament could be stretched (by optical tweezers, electric fields, elongational flows, ...), but it could also be quenched, i.e., prepared in an initial low-temperature environment. In all cases, the longitudinal contraction is driven by the same purely stochastic forces, yet the resulting deterministic growth laws for pertinent observables reflect for short times fundamental differences in the underlying relaxation processes. We present a comprehensive explanation how these differences emanate from the various realizations and how they give rise to universal long-time relaxation. Further, we compare our theoretical results to recent experiments and simulations, give suggestions on how to test our predictions, and comment on the choice of proper observables.