

## Semiflexible Polymers and Filaments



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Thesis: Strings and Filaments:

From Vortices to Biopolymers

Many biopolymers such as DNA, filamentous (F-) actin or microtubules belong to the class of semiflexible polymers. The biological function of these polymers requires considerable mechanical rigidity. For example, actin filaments are the main structural elements of the cytoskeleton in which actin filaments form a network rigid enough to maintain the shape of the cell and to transmit forces, yet flexible enough to allow for cell motion and internal reorganization in response to external stimuli. Synthetic semiflexible polymers also play an important role in chemical physics. Prominent examples are polyelectrolytes or dendronized polymers, where the electrostatic repulsion of charges along the backbone or the steric interaction of side groups gives rise to considerable bending rigidity.

The bending rigidity of semiflexible polymers is characterized by their persistence length [1], which is given essentially by the ratio of bending rigidity  $\kappa$  and thermal energy. The physics of semiflexible polymers becomes qualitatively different from the physics of flexible synthetic polymers on length scales smaller than the persistence length where bending energy dominates over conformational entropy. Typical biopolymer persistence lengths range from 50nm for DNA to the 10m-range for F-actin or even up to the mm-range for microtubules and are thus comparable to typical contour lengths such that semiflexible behaviour plays an important role.

We theoretically investigate the physics of semiflexible polymers and filaments from the single polymer level to biological structures consisting of assemblies of interacting filaments. This requires exploring the interplay of thermal fluctuations, external forces, interactions, and active fluctuations in filament systems.

### Single Filaments:

#### Fluctuations, Confinement, and Manipulation

The persistence length of a semiflexible polymer gives a typical length scale for its thermal shape fluctuations. The bending energy couples shape fluctuations of different wavelengths. Using a functional renormalization group approach, we calculated how this results in a softening of the polymer with an exponential decay of its bending rigidity for large wavelength fluctuations. This effect provides a concise definition of the persistence length as the characteristic decay length of the bending rigidity [1].

Thermal fluctuations of confined filaments are not only characterized by their persistence length but also by the so-called deflection length, which is related to the confining geometry. In a recent study [2] we performed a quantitative fluctuation analysis for actin filaments confined to microchannels and determined both persistence and deflection length.

During the last decade, micromanipulation techniques such as optical tweezers and atomic force microscopy (AFM) have become available which allow the controlled manipulation of single polymers and filaments. Experiments such as pulling single polymers or pushing adsorbed polymers over a surface with an AFM tip open up the possibility of characterizing mechanical filament properties on the single molecule level. In order to interpret such experiments quantitatively, theoretical models are necessary, which we developed for (i) force-induced desorption or unzipping of filaments [3] and (ii) the activated dynamics of semiflexible polymers on structured substrates [4,5].

AFM tips or optical tweezers can be used to lift an adsorbed semiflexible polymer from a surface or unzip two bound semiflexible polymers (Fig.1). We can calculate the resulting force-extension characteristics for such a force-induced desorption process [3]. One interesting feature is the occurrence of an energetic barrier against force-induced desorption or unzipping which is solely due to the effects from bending rigidity (Fig.1).

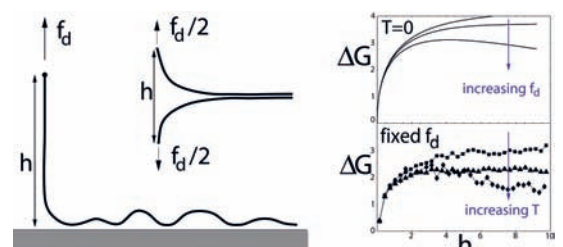


Fig. 1: Left: Force-induced desorption of an adsorbed filament and unzipping of two bound filaments. Right: Free energy landscapes for force-induced desorption as a function of the height  $h$  of the polymer end. The polymer desorbs either upon increasing the desorbing force  $f_d$ , or the temperature  $T$ . Both processes are governed by a free energy barrier.

Strongly adsorbed polymers are often subject to surface potentials that reflect the symmetry of the underlying substrate and tend to align in certain preferred directions. If such polymers are pushed over the substrate by point forces as can be exerted by AFM tips, their dynamics is thermally activated and governed by the crossing of the surface potential barriers. Barrier crossing proceeds by nucleation and subsequent motion of kink-antikink pairs (Fig.2). The analysis of this process shows that static and dynamic kink properties are governed by the bending rigidity of the polymer and the potential barrier height [4,5].

Structured adsorbed surfaces can also give rise to confinement effects that result in morphological shape transitions of single semiflexible polymers. Currently, we are investigating the morphological diagram for semiflexible polymer rings on a structured substrate containing an adhesive stripe (Fig.2). Upon increasing the adhesive potential of the stripe the polymer undergoes a morphological transition from an elongated to a round conformation.

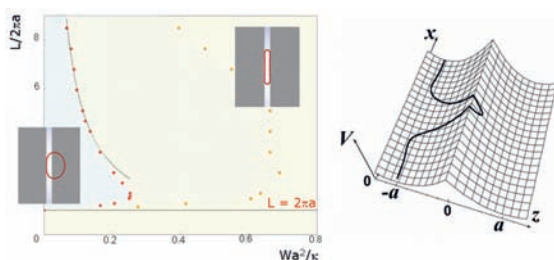


Fig. 2: Right: Kinked conformation of a semiflexible polymer, which is pushed at its mid-point over a potential barrier. Left: Morphological diagram of a semiflexible polymer ring adsorbed on a substrate containing an adhesive stripe of width  $a$  as a function of the polymer length  $L$  and the ratio of adhesive strength of the stripe and the polymer bending rigidity. In the red region at high adhesive strength, the ring assumes an elongated conformation within the stripe; in the blue region it exhibits a round conformation dominated by bending energy.

### Filament Assemblies

Filament assemblies play an important role as functional and structural elements of the cytoskeleton. Using analytical and numerical methods we studied the formation of filament bundles. In the cell, filament bundles are held together by adhesive crosslinking proteins. In a solution of crosslinkers and filaments, the crosslinkers induce an effective attraction between filaments. Starting from analytical results for  $N$  filaments, we have studied this problem analytically for  $N$  filaments and numerically for up to 20 filaments using Monte-Carlo simulations [6]. Above a threshold concentration of crosslinkers a bundle forms in a discontinuous bundling phase transition [6]. This mechanism can be used by the cell to regulate bundle formation. Deep in the bundled phase at high crosslinker concentration, we observe a segregation of bundles into smaller sub-bundles, which are kinetically arrested (Fig. 3). The system appears to be trapped in a glass-like state. Starting from a compact initial state, on the other hand, the bundle reaches its equilibrium configuration with a hexagonal arrangement of filaments (Fig. 3).

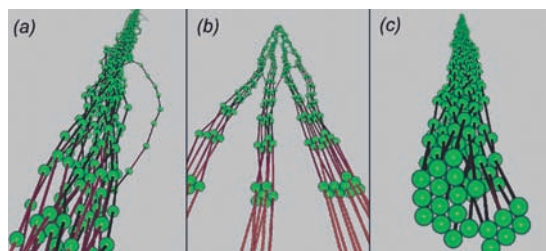


Fig. 3: Three snapshots of a bundle formed by twenty filaments as observed in computer simulations: (a) Loose bundle for a crosslinker concentration that is only slightly above the threshold value; (b) and (c) show two different conformations of the same bundle corresponding to a segregated conformation with three sub-bundles and a compact conformation with roughly cylindrical shape, respectively.

### Active Filament Systems

The living cell is an active system where cytoskeletal filaments are not in equilibrium. ATP- or GTP-hydrolysis allows them to constantly polymerise and de-polymerise (treadmilling). For filament bundles, this active polymerisation dynamics can be used for force generation. We found that filament bundles can generate polymerization forces but also zipping forces by converting the gain in adhesive energy upon bundling into a force exerted on a confining wall [7].

Cytoskeletal filaments also interact with molecular motors, which are motor proteins walking on filaments by converting chemical energy from ATP-hydrolysis into mechanical energy. The interplay between filaments and molecular motors can give rise to structure formation far from equilibrium. This can be studied in model systems such as motility assays where motor proteins are immobilized onto a glass plate and actively pull filaments over this surface. Computer simulations and theoretical arguments show that the active driving by molecular motors enhances the tendency of filaments to align: As one increases the density of molecular motors, the system undergoes a phase transition into a nematic liquid crystal (Fig. 4) [8,9]. This ordering effect arises from the interplay of the active driving by molecular motors and steric interactions between filaments. We were able to describe the resulting phase diagram of this non-equilibrium filament system quantitatively in terms of experimentally accessible model parameters by introducing the concept of an effective increased filament length [8]. The density of inactive motors and microscopic motor parameters such as detachment and stall forces determine the formation of a new non-equilibrium phase, a kinetically arrested cluster phase with mutually blocking filaments [9].

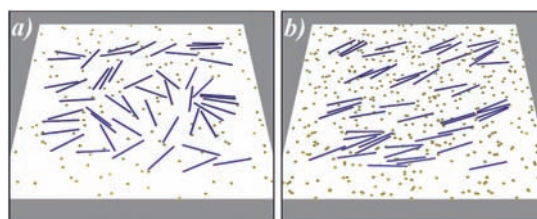


Fig. 4: Two snapshots of rodlike filaments (blue) on a surface coated with immobilized molecular motors (yellow). (a) At low motor surface density the filaments display no order. (b) Above a threshold value for the motor density, the filaments spontaneously order into a parallel pattern. This "active nematic ordering" is caused by the interplay of filament collisions and their motor-driven motion.

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