

Semiflexible Polymers and Filaments



Many biopolymers such as DNA, filamentous (F-) actin or microtubules belong to the class of semi-flexible polymers. The biological function of these polymers requires considerable mechanical rigidity. For example, actin filaments are the main structural element of the cytoskeleton which gives the cell unique mechanical properties as it forms 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 mechanical stimuli. Another important class of semi-flexible polymers are polyelectrolytes where the electrostatic repulsion of the charges along the backbone can give rise to considerable bending rigidity depending on the salinity of the surrounding solution.

The physics of semi-flexible polymers becomes fundamentally different from the physics of flexible synthetic polymers when their bending energy dominates over conformational entropy. The bending stiffness is characterized by the persistence length. On scales smaller than the persistence length, bending energy dominates and qualitatively new semi-flexible behaviour appears. Biopolymer persistence lengths range from 50nm for DNA to the 10 μ m-range for F-actin or even up to the mm-range for microtubules and are thus comparable to typical contour lengths such that semi-flexible behaviour plays an important role.

Binding and Adsorption

Binding of two polymers and adsorption of a polymer onto a surface (Fig. 1) are two phase transitions of fundamental importance. For both transitions, semi-flexibility is relevant and leads to new critical exponents, or changes even the order of the transition [1,2]. In contrast to flexible polymers, binding and adsorption transitions of semiflexible polymers are typically *discontinuous*. Semiflexible polymers bind or adsorb more easily the more rigid they are.



Fig. 1: Left: Binding of two polymers, Right: Adsorption onto an adhesive surface.

Single Polymer Manipulation

During the last decade micromanipulation techniques such as optical tweezers and atomic force microscopy (AFM) have become available which allow a controlled manipulation of single polymers and filaments. Experiments such as stretching of single DNA 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 experiments quantitatively, theoretical models are necessary which allow to calculate the response of a polymer to external forces. We investigated such models for (i) the stretching of semiflexible harmonic chains [3], (ii) the activated dynamics of semiflexible polymers on structured substrates [4,5], and (iii) force-induced desorption.

(i) In order to improve the quantitative interpretation of force-extension curves from stretching experiments on single semiflexible polymers such as DNA or F-actin, we introduced a semiflexible harmonic chain model [3]. This model includes not only the bending rigidity, but also takes into account the polymer extensibility, the monomer size and the finite contour length. Our results for this model allow to extract all of these parameters from experimental force-extension curves. (ii) 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 a homogeneous force arising, e.g., from hydrodynamic flow or by a point force 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], which implies that experimental measurements of the kink properties can be used to characterize material properties of both the semiflexible polymer and the substrate.

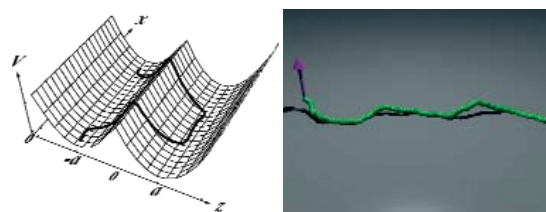


Fig. 2: Left: Kinked conformation of a semi-flexible polymer in a double-well potential. Right: Snapshot of a Monte-Carlo simulation of an adsorbed polymer. A force applied to one polymer end (arrow) can lead to force-induced desorption

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(iii) AFM tips can also be used to lift an adsorbed polymer from a surface (**Fig. 2**). We can calculate the resulting force-extension characteristics for such a force-induced desorption process. One interesting feature is the occurrence of an energetic barrier against force-induced desorption which is solely due to the effects from bending rigidity.

Filament Bundles

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 and numerically for up to 20 filaments using Monte-Carlo simulations [6], 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**).

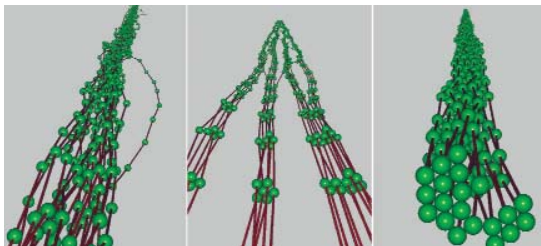


Fig. 3: Monte-Carlo snapshots of filament bundles.

Left: Close to the bundling transition.

Middle: Deep in the bound phase bundles tend to segregate.

Right: Equilibrium shape of the bundle.

Active Filaments

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). The active polymerisation dynamics can be used for force generation. Extending our work on filament bundles, we study force generation by growing filament bundles.

Cytoskeletal filaments not only generate force by active polymerisation but 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 filaments are adsorbed and actively transported over a glass plate, which is covered with anchored molecular motors. Computer models of such assays allow to predict and quantify formation of filament patterns, e.g., clustering and ordering (**Fig. 4**). Apart from motor and filament densities, also microscopic motor parameters such as their stall and detachment force determine the emerging pattern and can thus be inferred from the experimentally observed filament structures.

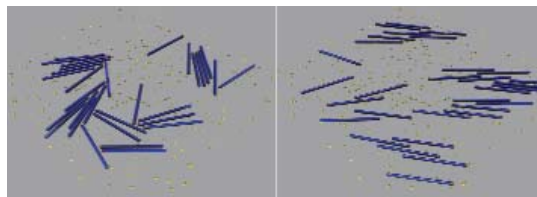


Fig. 4: Snapshot of a motility assay simulation. Filaments (blue) are driven by molecular motors (yellow) over a substrate (grey).

Left: Formation of immobile clusters of filaments blocking each other.

Right: Nematic ordering due to collisions of moving filaments.

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