

Semiflexible Polymers and Filaments



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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 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 transmit forces yet flexible enough to allow for cell motion and internal reorganization as response to external mechanical stimuli.

The physics of semiflexible polymers is in many respects fundamentally different from the physics of flexible synthetic polymers such as polyethylene.

For semiflexible polymers not only the conformational entropy but also the bending energy plays an important role. The bending stiffness is characterized by the persistence length. On scales larger than the persistence length the polymer loses its orientation and starts to behave as flexible, mostly entropic chain whereas on smaller scales bending energy dominates and qualitatively new semiflexible behavior appears. The persistence lengths of the most prominent biopolymers range from 50 nm for DNA to the 10 μm -range for F-actin or even up to the mm-range for microtubules and are thus comparable to typical contour lengths the polymers such that semiflexible behavior plays an important role.

Another important class of semiflexible polymers are polyelectrolytes where the electrostatic repulsion of charges along the backbone can give rise to considerable bending rigidity depending on the salinity of the surrounding solution.

Semiflexibility is also crucial for the bundling of two such biopolymers by attractive interactions as well as their adsorption onto adhesive substrates as shown schematically in **Fig. 1**. Unbundling and desorption transitions are due to the competition between the energy gained by binding to an attractive potential well and the associated loss of configurational entropy. As the bending rigidity and, thus, the persistence length is increased the entropy loss is reduced. Therefore semiflexible polymers bundle and adsorb more easily as compared to a flexible polymer.

These problems can be theoretically described as single polymer problems in the presence of an external binding or adsorbing potential. Intermolecular forces give rise to polymer/polymer or polymer/surface interactions that contain both an attractive potential well and a repulsive hard core, see **Fig. 2**. However, attraction might also depend on the orientation of polymer segments, for example, if the binding is mediated by crosslinkers.

We have studied this problem analytically solving the differential transfer matrix equation **[1]**. The transfer matrix calculation allows to obtain explicit expressions for the transition points, the order of the unbundling and desorption transition, and the critical exponents which characterize the corresponding critical behavior. Results for the critical exponents agree with renormalization group results **[2]**. The transfer matrix approach identifies up to four distinct universality classes corresponding to the four interaction potentials shown in **Fig. 2**. Somewhat surprisingly, it turns out that the orientation dependence of the attraction can influence the order of these transitions which is a distinct feature of semiflexible polymers. In 1+1 dimensions the transfer matrix approach even allows to calculate the exact distribution of polymer segment positions and orientations. We also find that the repulsive hard core part of the interaction potential becomes irrelevant in higher dimensions $d \geq 3$. All analytical results have been confirmed by numerical transfer matrix calculation and Monte-Carlo simulations, a snapshot of which is shown in **Fig. 3**.

Desorption does not only occur as a result of increasing temperature and thermal fluctuations but also if a desorbing force is applied to one end of the polymer, as indicated in **Fig. 3**. This force-induced desorption can be experimentally studied using single molecule AFM techniques. Using the exact transfer matrix result for the probability distribution of polymer segments the force-extensions characteristics for desorption by an applied force can be obtained. One interesting feature is the occurrence of an energetic barrier against force-induced desorption which is solely due to the effects from bending rigidity.

A bundle of three attractive semiflexible polymers (**Fig. 4**) represents a more challenging problem that can only be studied by scaling arguments and extensive Monte-Carlo simulations **[3]**. One basic question regarding bundles of more than two polymers is whether the bundling proceeds via a sequence of transitions in pairs or in a single cooperative transition. Surprisingly it turns out that the phase transition is cooperative, similar to what is shown in **Fig. 5** for identical persistence lengths, even for a wide range of different persistence lengths.

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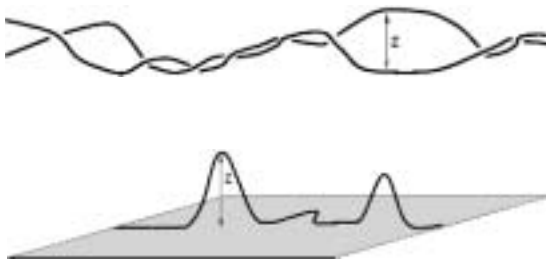


Fig. 1: Top: Bundling of two semiflexible polymers. Bottom: Adsorption of a semiflexible polymer onto a planar substrate.



Fig. 4: Snapshot of a Monte-Carlo simulation of a bundle of three semiflexible polymers.

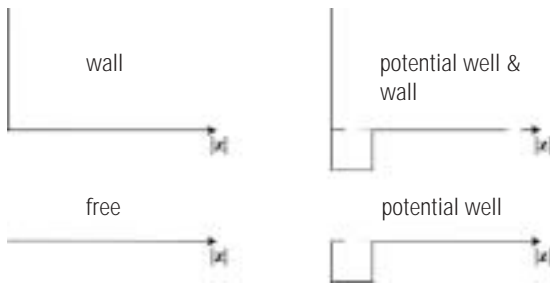


Fig. 2: Four types of interaction potentials corresponding to the four different universality classes.



Fig. 3: Snapshot of a Monte-Carlo simulation of an adsorbed polymer. A force applied to one polymer end (arrow) can lead to force-induced desorption.

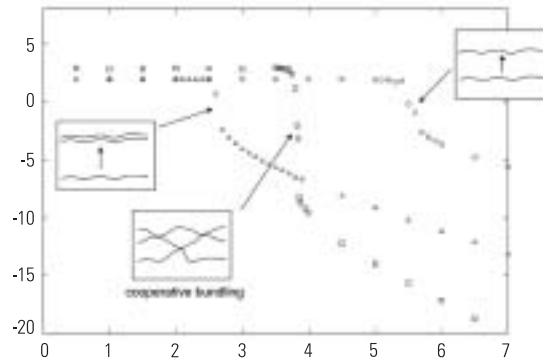


Fig. 5: Potential energy of three identical semiflexible polymers as function of attraction strength in 1+2 dimensions. The discontinuity signals the location of a (first order) bundling transition. Two subsequent transitions in pairs would give the curves on the right (circles) and on the left (triangles). The Monte-Carlo simulation shows that the actual transition is cooperative and happens along the curve in the middle (squares) before the first pair can bind.

References:

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