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Historical perspective

## Bundling in semiflexible polymers: A theoretical overview

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## ABSTRACT

Supramolecular assemblies of polymers are key modules to sustain the structure of cells and their function. The main elements of these assemblies are charged semiflexible polymers (polyelectrolytes) generally interacting via a long(er)-range repulsion and a short(er)-range attraction. The most common supramolecular structure formed by these polymers is the bundle. In the present paper, we critically review some recent theoretical and computational advances on the problem of bundle formation, and point a few promising directions for future work.

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## 1. Introduction

Many important biomolecules, including the structural elements of the cytoskeleton (F-actin, microtubules, and intermediate filaments), are semiflexible polymers, that is their physical behavior is dominated by their resistance to bending which gives rise to a finite-persistence length of their backbone orientation. These semiflexible

polymers form polymorphous supramolecular self-assembled structures resulting from the interplay of energetic and entropic contributions. Prominent among them are the bundles. These are assemblies of relatively closely packed, parallel aligned semiflexible filaments. It has been shown that their conformational and mechanical behavior is fundamentally different from that of a single filament [1]. As such, they play an important role in various biological functions, optimizing adaptability and mechanical performance. They may also prove useful in biomimetic applications [2]. Theoretically understanding their properties and formation is a challenging task because it combines the complexity of the single filament with that of the many-body problem. Another subtlety which complicates the

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theoretical analysis of bundles is the precise identification of the bundled state by means of an order parameter. Bundles involve alignment of polymers, but they differ from a simple polymer nematic phase. The latter is translationally uniform in the plane transverse to the alignment direction, whereas polymers in bundles are more densely packed compared to their neighbors outside. This is related to the major question of the mechanism behind the fact that most experimentally observed semiflexible bundles have a finite width.

In this critical review, we summarize the main theoretical approaches to the problem of bundle formation in systems of semiflexible polymers. We try to clearly state the main assumptions underpinning various models and compare their relative strengths and weaknesses, emphasizing their complementary merits. Our main focus is on analytic works, but we also include a section on numerical simulations since the latter serve as a bridge to experiments. As bundling requires an attractive interaction between filaments, usually involving cross-linking molecules, we present the theoretical treatment of permanent (chemical) cross-links in Section 2.1 and that of reversible (physical) cross-links in Section 2.2. The latter, under certain conditions, correspond to an effective pairwise attractive potential. This attraction, in most semiflexible biopolymers, competes with the electrostatic repulsion of like-charged macroions. Because of the important role of electrostatics in the bundling of semiflexible polyelectrolytes, we devote Section 2.3 to survey the main ideas. In Section 3, we review the key papers on system-specific mechanisms of finite-size bundle formation (inherent helicity, quenched packing defects, charge fluctuations). Section 4 is about the main strategies of numerical simulations for these systems.

We point out that this paper is not meant as a comprehensive overview of all works relevant to self-assembled structures of semiflexible polymers. We apologize to the colleagues whose work is not mentioned, and we refer the interested reader to some recent review articles which cover important aspects unavoidably left out of our survey. The review by Broedersz and MacKintosh includes sections on the statistical mechanics of a single semiflexible chain, on affine and non-affine deformations of semiflexible polymer networks, as well as on marginally stable fibrous systems [3]. Pritchard et al. review several key in vitro and in vivo experiments on cytoskeletal biopolymers and focus on the elasticity of polymer networks up to the level of tissue [4]. Lieleg et al. review the structural polymorphism of emerged structures in F-actin networks cross-linked through a variety of different cross-linkers [5]. Grason reviews the physics of closely packed filaments and its relation to the packing on positively curved surfaces (Thomson problem) [6]. Popp and Robinson summarize the formation of supramolecular structures by cellular filaments with emphasis on the specific features of the various semiflexible biopolymers which are involved [7].

## 2. Theoretical models of bundle formation

### 2.1. Permanent cross-links

Permanent cross-links can be treated as geometrical constraints. They have been approached from the point of view of gelation theory in anisotropic macromolecular networks in Refs. [8,9,10,11]. The original system consists of  $N$  identical wormlike chains of contour length  $L$  and persistence length  $L_p$  in 3d parametrized by  $\mathbf{r}_i(s), i = 1, 2, \dots, N, s \in [0, L]$  with a Hamiltonian:

$$\mathcal{H}(\{\mathbf{r}_i(s)\}) = \sum_{i=1}^N \frac{1}{2} \kappa \int_0^L ds (\partial_s \mathbf{t}_i(s))^2 + \sum_{ij=1}^N \frac{1}{2} \lambda^2 \int_0^L ds \int_0^L ds' \delta[\mathbf{r}_i(s) - \mathbf{r}_j(s')] \quad (1)$$

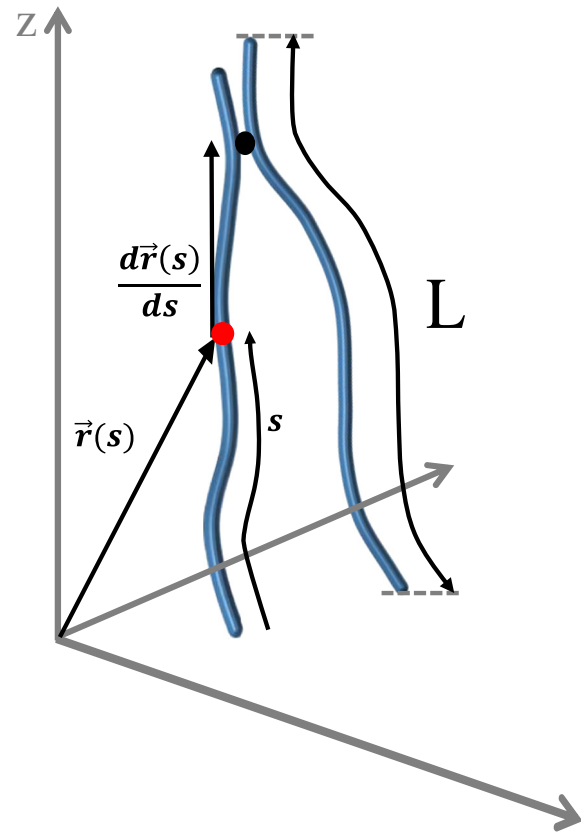


Fig. 1. Schematics: the position vector  $\mathbf{r}(s)$ , tangential vector  $\mathbf{t}(s) \equiv \frac{d\mathbf{r}(s)}{ds}$ , and the arclength positions are defined graphically. The black dot indicates the cross-link.

$M$  chemical (permanent) cross-links are introduced simultaneously and instantaneously in such a way that (a) “glue” together the corresponding segments and (b) align them to be parallel or antiparallel, as shown in Fig. 1.  $\mathbf{t}_i(s)$  is the tangent vector at arclength position  $s$  of polymer  $i$ ,  $\kappa$  is the bending rigidity (determining the persistence length via  $L_p = 2\kappa/(k_B T)$ ), and  $\lambda^2$  expresses an excluded-volume interaction à la Edwards.

Quenched disorder refers to the network structure imposed by the cross-linking constraints. This structure is determined by specifying the number of cross-links  $M$ , the constrained polymer segments, and the parallel or antiparallel way to align the corresponding tangent vectors. The probability of a given cross-link conformation  $C_M$  is assumed to follow the Deam-Edwards distribution [12]:

$$\mathcal{P}(C_M) \propto \frac{1}{M!} \left( \frac{\mu^2 V}{N} \right)^M \left\langle \prod_{e=1}^M \delta(\mathbf{r}_{i_e}(s_e) - \mathbf{r}_{j_e}(s'_e)) \right\rangle, \quad (2)$$

where the parameter  $\mu^2$  controls the average number of cross-links:  $[M]/N \approx \mu^2$ . In the absence of the average (...), Eq. (2) would have been just a Poisson distribution controlling the average number of cross-links which could appear anywhere. The average (...) is calculated with the Boltzmann weight of the uncross-linked system. This factor in the Deam-Edwards distribution expresses the fact that polymer segments close to each other in the sol (uncross-linked phase) have a high probability of getting linked.

Physical observables are calculated from the quenched-disorder averaged free energy,  $F = -k_B T [\ln Z(C_M)] \propto \sum_{M=0}^{\infty} \sum_{\{C_M\}} \mathcal{P}(C_M)$

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