Tutorial 1: Entropic elasticity of a semiflexible filament

Physics of Complex Systems M2 – Biophysics

Long thin filaments are ubiquitous in the cell, be they DNA molecules, structural elements of the cytoskeleton made out of proteins or carbohydrates such as polysaccharides used for energy storage or selected for their material properties (*e.g.*, cellulose or chitin). In many cases, the mechanical response of these objects is crucial for their biological function, and is strongly influenced by thermal fluctuations.

Here we consider the response of a somewhat rigid polymer, *e.g.*, a DNA filament to a longitudinal pulling or pushing force [see Fig. 1, as well as the classic reference Marko & Siggia, *Macromolecules* **28**, 8759 (1995)]. This response is dominated by a spring-like elasticity that originates in the straightening out of its transverse fluctuations, as discussed in the following. We thus look for the force-extension relation of that nonlinear spring. While physically related, the three sections can be tackled independently.

1 Force-extension relation

We consider an almost rectilinear polymer lying along the z direction, and denote its small lateral displacement along the transverse directions x and y by $\mathbf{r}_\perp = \{x(z), y(z)\}$. In this representation, the energy of the polymer is primarily due to its bending stiffness, and thus depends on its local curvature $|\partial_z^2 \mathbf{r}_\perp| = \sqrt{(\partial_z^2 x)^2 + (\partial_z^2 y)^2}$. As further discussed in Sec. 3, the resulting bending energy reads

$$E_b = \int_0^S \left\{ \frac{k_B T \ell_p}{2} \left[\left(\partial_z^2 x\right)^2 + \left(\partial_z^2 y\right)^2 \right] \right\} \mathrm{d}z, \tag{1}$$

where ℓ_p is a constant known as the persistence length and the total length S of the filament is also constant. The action of the outside tensile force F pictured in Fig. 1 results in an additional energy

$$E_t = \int_0^S \left\{ \frac{F}{2} \left[\left(\partial_z x\right)^2 + \left(\partial_z y\right)^2 \right] \right\} \mathrm{d}z \tag{2}$$

Assuming that the filament is attached such that $\mathbf{r}_\perp(0) = \mathbf{r}_\perp(S) = \mathbf{0}$, we use the Fourier decomposition

$$\mathbf{r}_\perp(z) = \sum_{n=1}^{+\infty} \tilde{\mathbf{r}}_n \sin\left(\frac{n\pi z}{S}\right) \qquad \text{with} \qquad \tilde{\mathbf{r}}_n = \tilde{x}_n \hat{\mathbf{x}} + \tilde{y}_n \hat{\mathbf{y}}. \tag{3}$$

1.1 Write the total energy $E = E_b + E_t$ as a function of the Fourier components $\tilde{x}_n$ and $\tilde{y}_n$, making sure to perform the integrations over z to simplify the result.

1.2 Using the equipartition theorem, write the equilibrium thermal averages $\langle \tilde{x}_n \rangle$ and $\langle \tilde{x}_n^2 \rangle$.

1.3 As will be discussed in Sec. 3, the end-to-end length of the filament is given by

$$L = \int_0^S \sqrt{1 - \left[(\partial_s x)^2 + (\partial_s y)^2 \right]}\, \mathrm{d}s \simeq S - \frac{1}{2} \int_0^S \left[(\partial_z x)^2 + (\partial_z y)^2 \right] \mathrm{d}z \tag{4}$$

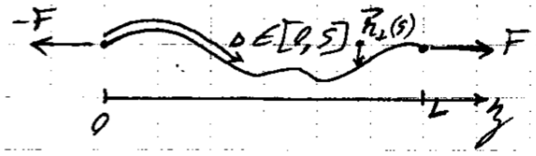

Figure 1: Parametrization of the filament. Here fluctuations take place in both the x and y directions.

to lowest order in the filament slope. Conclude from that that

$$\langle L\rangle \simeq S - \frac{S^2}{\pi^2 \ell_p}\sum_{n=1}^{+\infty}\frac{1}{n^2+\phi}, \tag{5}$$

where ϕ is the force F up to a normalization to be specified.

1.4 Prove that for $\zeta \geq 0$

$$\sum_{n=-\infty}^{+\infty}\frac{e^{in\zeta}}{n^2+\phi} = \frac{\pi}{\sqrt{\phi}}\left[\frac{e^{\zeta\sqrt{\phi}}}{e^{2\pi\sqrt{\phi}}-1}+\frac{e^{-\zeta\sqrt{\phi}}}{1-e^{-2\pi\sqrt{\phi}}}\right]. \tag{6}$$

1.5 Deduce from this the filament's force-extension relationship:

$$\langle L\rangle \simeq S - \frac{S^2}{\ell_p}\frac{\pi\sqrt{\phi}\coth(\pi\sqrt{\phi})-1}{2\pi^2\phi} \tag{7}$$

2 Discussion of the mechanical properties

2.1 What is the physical meaning of the persistence length ℓ_p? For DNA, $\ell_p \simeq 50\,\text{nm}$. For actin, $\ell_p \simeq 10\,\mu\text{m}$.

2.2 Draw the small-slope force-extension relationship of Eq. (7). What is the typical stiffness of the filament in the linear response regime? Its divergence denotes the buckling of the filament. What force is required to achieve this buckling? How large is it for a typical actin filament with $S \simeq 400\,\text{nm}$? How does it compare to the typical molecular motor force $\approx 1\,\text{pN}$? How much filament compression do you expect under such a force?

2.3 What happens beyond buckling? Give the scaling of the buckled filament's rigidity. Compare this situation with bending the filament with a transverse force.

3 Energy of a filament

We now study the foundation of the energies introduced in Sec. 1. We consider an inextensible filament with constant total arclength S, but whose end-to-end length L fluctuates (Fig. 1).

3.1 The molecular bonds between the monomers constituting the filament tend to keep it straight, and the local energy of the filament depends only on its local shape. Thus the filament bending energy can be expressed as

$$E_b = \int_0^S f[c(s)]\,\mathrm{d}s, \tag{8}$$

where $c(s)$ is the curvature of the filament at the location characterized by the arclength s and f is an unknown function. Expand f for a weakly deformed filament to obtain an explicit form for the bending energy as a function of $c(s)$ up to an unknown multiplicative constant. This so-called "worm-like chain model" is a staple of the study of biological semiflexible polymers.

3.2 For a curve defined by its position vector $\mathbf{r}(s)$, the curvature $c(s)$, tangent unit vector $\hat{\mathbf{t}}(s)$ and normal unit vector $\hat{\mathbf{n}}(s)$ are defined through

$$\hat{\mathbf{t}} = \partial_s \mathbf{r}; \qquad c\hat{\mathbf{n}} = \partial_s \hat{\mathbf{t}}. \tag{9}$$

Writing $\mathbf{r}(s) = \mathbf{r}_\perp(s) + z(s)\hat{\mathbf{z}}$, where $\mathbf{r}_\perp$ is a vector contained within the xy, show that to lowest order in the filament deviation from a straight line E_b is given by Eq. (1).

3.3 Prove Eq. (4).

3.4 Using this result and assuming the filament is being pulled at both ends by a force $\mathbf{F} = \pm F\hat{\mathbf{z}}$ as in Fig. 1, demonstrate that the energy E_t associated with the tension of the filament is given by Eq. (2).