Configurations of DNA molecules

Helmut Schiessel, Leiden University

DNA is a rather stiff polymer. Its mechanical properties can be well approximated by the wormlike chain model, that describes DNA as an elastic rod with fixed contour length and a local bending energy (per length) that is given by $(A/2)(1/R^2)$. Here A denotes the bending modulus of the rod and R the local radius of curvature.

The shapes of such rods under various boundary conditions have been worked out by Leonhard Euler in 1744, see Figure 1. These shapes, the so-called Euler elasticas, are described by elliptic functions that are difficult to deal with. A useful approximation that typically deviates only about 10% from the exact result is the circle-line approximation. One replaces the exact shape by a set of straight lines and sections of circles that are connected smoothly and minimizes the bending energy with respect to some free parameter. As example consider one half of the lying figure 8 that Euler happened to call Fig. 8 (see Figure 1). One obtains this shape when one bends a beam such that its two ends touch, a relevant problem in gene regulations that involves DNA looping. From a numerical minimization one finds that the apex angle at the tip is given by 81.6°.

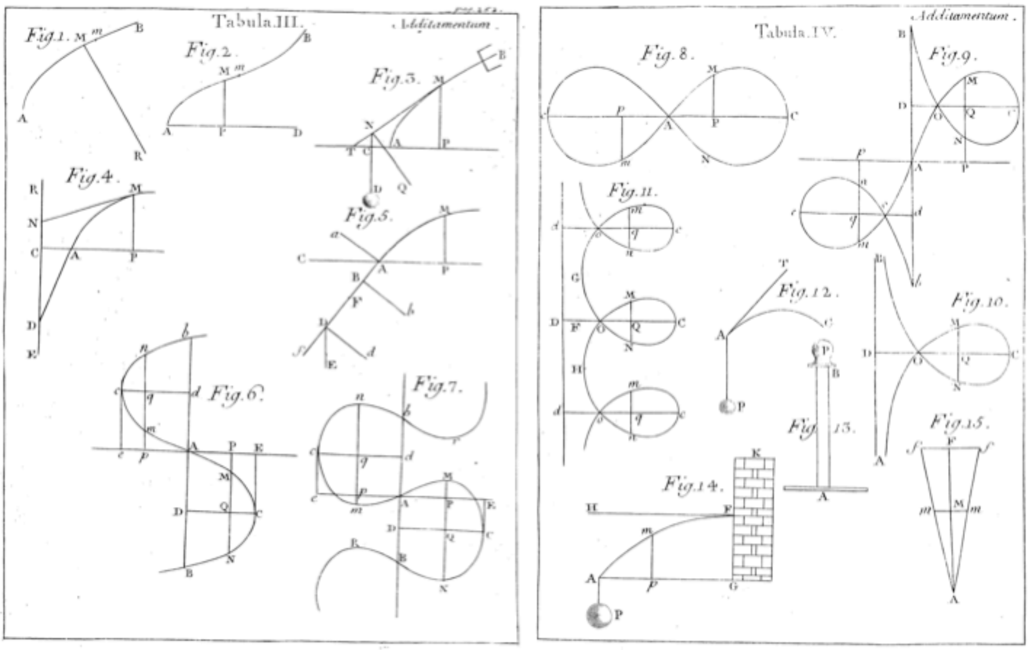

Figure 1: Euler's 1744's drawings of the elasticas

[1] Estimate this angle using a circle-line approximation. You can approximate the tear-shaped loop by two lines that touch at one end and are connected via a circular section at the other end. Assume that the total length of the two lines plus that of the circle is fixed to L. Minimize the bending energy (only the circular part is bent with a constant curvature) with respect to the apex angle. Show that this leads to the transcendental equation $\pi + \alpha = \tan\alpha$ for the tip angle (this is solved for $\alpha = 77.5°$).

We consider next a free DNA molecule, i.e. a molecule without any constraints, but account for thermal fluctuations. One can show that in the thermal average – as a consequence of the above mentioned mechanical properties – the tangent-tangent correlations decay exponentially with the distance along the chain: $\langle \mathbf{t}(s_0)\cdot \mathbf{t}(s_0+x)\rangle = e^{-x/l_P}$ where $l_P = A/k_B T$ is called the *persistence length* ($k_B T$ is the thermal energy). Figure 2 shows the special case $x = l_P$ and states the actual value of l_P for DNA.

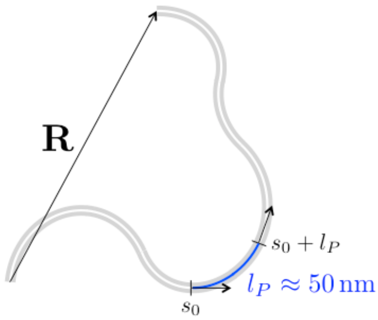

Figure 2: Configuration of a wormlike chain

[2] Calculate $\langle R^2\rangle$. (Hint: Use $\mathbf{R} = \int_0^L \mathbf{t}(s)\,ds$ where L denotes the total contour length of the chain).

We compare the above case now to the case of perfectly flexible polymers that have an enormous number of configurations, all with the same energy. A standard polymer model is the *freely jointed chain*: a chain consisting of *N* links, each of length *b* and able to point in any direction independently. A given configuration is then fully characterized by the set of bond vectors $\{\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N\}$ (see Figure 3).

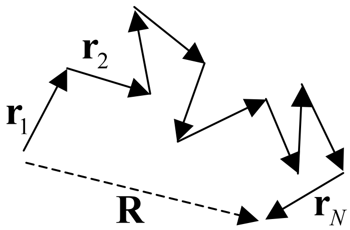

Figure 3: The freely jointed chain

[3] Determine for this polymer model the mean-squared end-to-end distance $\langle R^2\rangle = \langle \mathbf{R}^2\rangle = \left\langle \left(\sum_{i=1}^N \mathbf{r}_i\right)^2\right\rangle$. (Hint: Use the facts that each bond has a fixed length, $\langle \mathbf{r}_i^2\rangle = b^2$, and that different bonds are independent from each other, $\langle \mathbf{r}_i\cdot \mathbf{r}_j\rangle = 0$ for $i \neq j$).

[4] Long wormlike chains with $L >> l_P$ look on large length scales like flexible chains. Show this by comparing the expressions for $\langle R^2\rangle$ from [2] and [3].