

33-767, SS 2019, HW 4 (Feb-27, 2019)
due: Mar-06, 2019 (by e-mail: quench@cmu.edu)

Solve problems 8.9 and 8.11 in the textbook by Phillips *et al.* For students who do not own a copy, here are the statements of the problems. ***Please use a plot program for graphics (i.e., no hand-drawn graphs!).***

(1) Random Walk models for force-extension curves: Freely jointed chain in three dimensions (15 pts)

(a) Derive Eqn. 8.69 in Phillips *et al.*, which gives the extension of a polymer with Kuhn length a whose conformation resembles a random walk in 3 dimensions under an external force $f = -\partial G / \partial L$, where $G = -k_B T \ln W(L; L_{tot})$ and L_{tot} is the contour length:

$$z = \frac{\langle L \rangle}{L_{tot}} = \frac{2 \sinh(\beta f a)}{4 + 2 \cosh(\beta f a)}.$$

Start by assuming that each segment independently decides which way to point in one of the six Cartesian directions, $\mathbf{e}_1, -\mathbf{e}_1, \mathbf{e}_2, -\mathbf{e}_2, \mathbf{e}_3$ and $-\mathbf{e}_3$, and find the expected length $\langle L_0 \rangle$ in the direction of f . Use the result to derive the relation between force and extension, and make a plot of the resulting function.

(b) In the small-force limit, the force–extension curve is linear (see Fig. 1); that is, in this regime, the polymer behaves like an ideal Hookean spring with a stiffness constant $k \propto k_B T / L_{tot} a$. Demonstrate this claim and deduce the numerical factors that replace the proportionality with a strict equality.

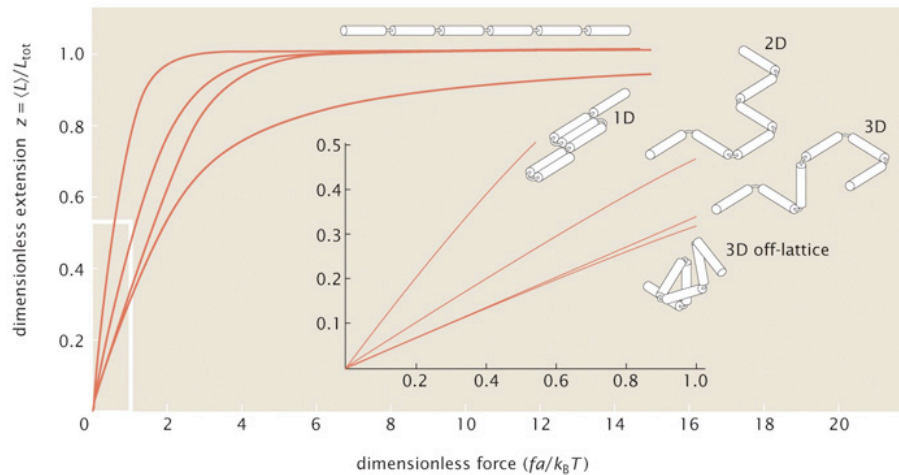


Figure 1: Force-extension relation obtained using the freely jointed chain model. The region in the white box is expanded in the inset. A comparison of the model prediction with actual data is shown in Fig. 5.14, p. 207 of the text.

(2) Transition between B and S form DNA

(15 pts)

DNA subjected to a stretching force exceeding 60 pN undergoes a structural transition from the usual *B* form to the so-called *S* form (“*S*” for stretched). Here we examine a simple model of this transition based on the freely jointed chain model of DNA and compare it with experimental data.

(a) Consider the freely jointed chain model in one dimension. Each link of the polymer points in the positive or negative x direction. There is a force f in the $+x$ direction applied at one of the ends (see Fig. 2).

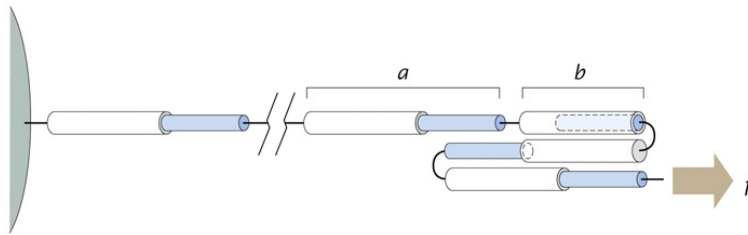


Figure 2: Fig. 8.35A from Phillips *et al.*, *Physical Biology of the Cell*.

To account for the B to S transition, assume that links are of length b (B state) or a (S state), with $a > b$. Furthermore, there is an energy penalty ε of transforming the link from a B state to an S state. (This is the energy, presumably, for unstacking the base pairs.) Write down the expressions for the total energy and the Boltzmann factor for each of the four states of a single link.

(b) Compute the average end-to-end distance for one link. The average end-to-end distance for a chain of N links is N times as large.

(c) Plot the average end-to-end distance normalized by Nb (that is, the relative extension) as a function of force using the numbers appropriate for DNA, namely, $b = 100$ nm and $a = 190$ nm. To estimate ε , take the energy per base pair for transforming B DNA to S DNA to be $5 k_B T$ (the stacking distance between base pairs is $l \sim 0.33$ nm in B DNA). How does your plot compare with the original data (Bustamante *et al.*, *Nature* 421, 2003, 423, see Fig. 3)?

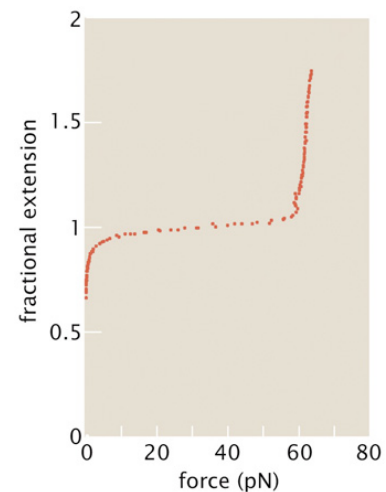


Figure 3: Actual data