

Problem 1

In class, we showed that the average end-to-end extension z of an ideal chain under tension f is given by

$$\frac{z}{L} = \left[\coth \frac{bf}{k_B T} - \frac{k_B T}{bf} \right]$$

where b is the statistical segment length of the chain, and $L = Nb$ is the total contour length.

(a) Plot the extension (z/L) as a function of the applied force for

- (i) double-stranded DNA ($b = 100$ nm)
- (ii) single-stranded DNA ($b = 3$ nm)
- (iii) denatured polypeptide ($b = 2$ nm).

(b) For what forces are these three types of polymers 50% extended?

Problem 2

Consider an ideal chain with $N = 1000$ statistical segments, each segment length $b = 0.5$ nm, carrying charges $\pm e$ at both ends (e is one electron charge). What will be its relative elongation (z/R_0) in a field $E = 30,000$ V/cm? Here z is the average end-to-end extension in the direction of the field, and R_0 is the root-mean-square end-to-end distance of the unperturbed chain.

Problem 3

- (a) Use the force extension relation of problem 1 to evaluate the work done in stretching a polymer. You may use numerical techniques to evaluate the integrals. This work is equal to the free energy of stretching.
- (b) Plot the free energy of the polymer versus extension.
- (c) Evaluate and plot the number of configurations accessible to the polymer at a given stretch relative to the number of configurations of the unperturbed polymer.
- (d) Compare your result in part (c) with a gaussian function

$$\frac{\Omega(z)}{\Omega(R_0)} = \exp\left(-\frac{3z^2}{2Nb^2}\right)$$

Problem 4

The free energy cost of bringing two ends of a semiflexible polymer of $L = na$ (where n is the number of monomers, and a is the size of each monomer) can be approximated as

$$F(n) = \frac{3k_B T}{2} \ln n + \frac{2\pi^2 g_b}{n}$$

Here $\frac{1}{2} g_b \theta^2$ is the energy cost of tilting the orientation of one monomer relative to the adjacent one by an angle θ .

- (a) Can you explain the origin of the two terms in the free energy?
- (b) Estimate g_b for
 - (i) double-stranded DNA for which the optimal loop size occurs at $n \approx 300$
 - (ii) single-stranded DNA for which the optimal loop size occurs at $n \approx 5$
- (c) Estimate the magnitude of the orientational fluctuation between successive monomers from thermal fluctuations.