Molecular, Cellular & Tissue Biomechanics, Fall 2006

20.310/2.797J/6.024J/

Problem Set # 2

Problem 1: Thermal Energy as a Ruler: In class we saw the probability that an interaction with energy E will break due to thermal energy kT is given by:

$$p(E) := \exp\left(\frac{-E}{kT}\right).$$

Plot this function over a range from 0.01 to 10kT. At what energies do we have 90% of bonds broken? half of bonds broken? 10% of bonds broken?

Problem 2: Calculate the energy of a hydrogen bond with partial charges of 0.8, 0.4 and a separation of 1.8 angstroms due to coulombic interactions. Assume both a dielectric constant of 1 and that for water. Now calculate the Bjerrum length for this interaction. Use the Bjerrum length to estimate a typical force magnitude required to break this interaction.

Problem 3: The physiological concentrations of ions in a cell are close to 150mM. Say you are making an artificial cell by creating lipid vesicles using $CaCl_2$ at 150mM to form an ionic solution. Calculate the Debye screening length in your artificial vesicle based cell.

Problem 4: Derive the $1/r^n$ dependence of the potential energy of interaction between two dipoles oriented along a line, pointing in the same direction.

Problem 5: The two structures below show two configurations of RNA. Loop formation in RNA can contribute an energetic cost of 7-8 kT for loops of 6-7 bases terminated in a G-C interaction. Note the G-C interaction, which is favorable, is counted in the loop structure's energetic "cost". Lets assume an unfavorable energy of 10kT for the loops found below, since they are slightly bigger or smaller than the optimal loop size. Also assume that in the structure on the left, there is no extra energetic cost for unpaired bases not part of loops. Finally assume the favorable energetic interaction for an A-U interaction is similar to A-T. Which structure is more stable and what are the relative populations of the two from the Boltzmann distribution?

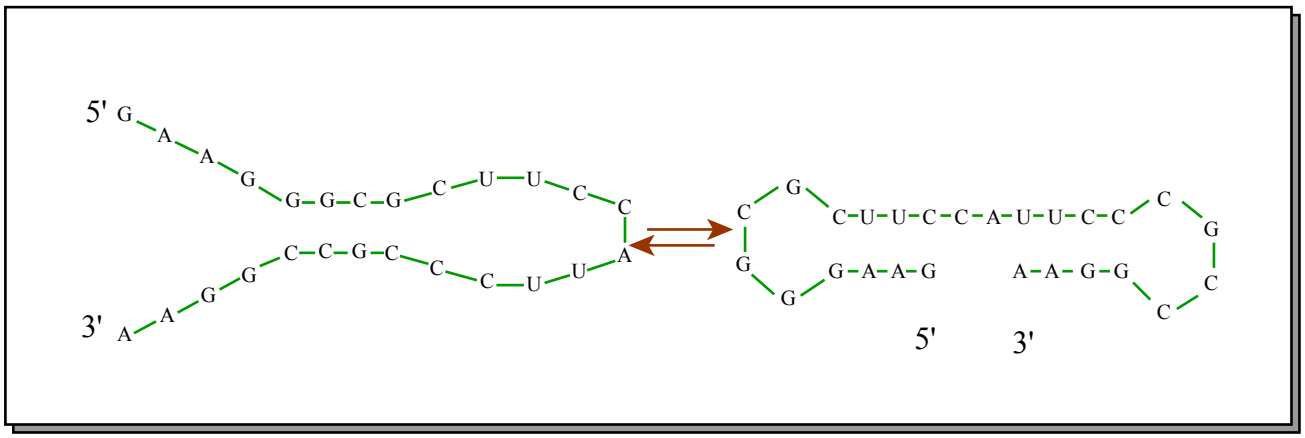
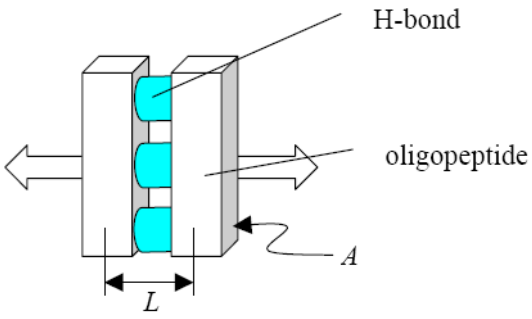


Figure by MIT OCW.

Problem 6:

Consider the simple case of two oligopeptides (short linear proteins) that are bound to each other by a series of 3 identical hydrogen bonds as shown schematically below.



Each bond can be treated as a linear spring such that the force exerted varies according to:

$$F = k(x - x_0)$$

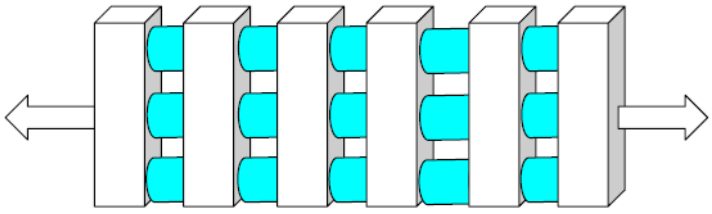
where k is the effective "spring stiffness" and x_0 the zero force position.

a) Find an expression for the energy stored in the spring as a function of k and the distortion, x-x_0.

b) If we assume that the change in stored energy in each bond is 10 k_BT, when $x = 2x_0$, can you find an expression for the spring constant k?

c) Find the total force generated by all three bonds when $x = 2x_0$.

d) If the cross-sectional area of the peptide is A, and the center-to-center distance in the relaxed state is L (see sketch), what is the effective elastic modulus, E, of a filament made from many of these peptides arranged side-by-side and stretched in the direction shown by the arrows in the sketch?



e) Using the values: x_0 – 0.2 nm, L = 4 nm, T = 300 degree K, calculate E.

Note the Elastic modulus is defined by the stress over the strain. $E=\sigma/\varepsilon$, where the stress, σ = Force/Area and strain, ε = change in length/total length L.