Molecular Biophysics, Physics 177, Spring 2008

Homework #2: Chain Statistics

Assigned February 14, 2008.

Due 5 PM February 22, 2008 to Birge 225.

1. The *characteristic ratio* of a polymer is defined as:

$$C_N = \langle h^2 \rangle / N\, l^2$$

which relates the mean square end-to-end distance h^2, the number of segments in the polymer, N, and the length of the segment, l. For a freely rotating chain (fixed θ, free ϕ) show that

$$C_4 = 1 + (6\alpha + 4\alpha^2 + 2\alpha^3)/4$$

where $\alpha = \cos\theta$. The characteristic ratio is important because it is a measure of the stiffness of the chain. Notice that for a freely jointed chain (FJC) $C_N = 1$, for all values of N. For real, stiffer, chains, C_N adopts an asymptotic value C, usually greater than 1.

2. The characteristic ratio C of polypeptides has been experimentally determined to be 10. Suppose that a polypeptide chain functions to link two organelles in the cell and maintain their distance at 50 Å. Use the FJC model to determine how many structural units there should be in the peptide so that, without tension or compression, an average end-to-end distance of 50 Å is maintained. Assume a virtual bond length of 3.8 Å. Compare the straightforward result of using $\langle h^2 \rangle$ with the number of structural elements that would be predicted by using the most probable h-value (h_{mp}) from the end-to-end distance distribution. Write the most probable value in terms of the number of statistical segments and the length.

3. Consider T4 DNA with a MW of 125 x 10^6 Daltons. Use the FJC model to calculate the volume per molecule, assuming a sphere of radius R_G. At what concentration of DNA (mg/ml) does the volume of the DNA spheres equal that of the solution? (Assume tightly packed spheres that exclude the solvent.) What do you predict will happen to the solution? Rationalize your answer in terms of the non-ideal behavior of real polymers.

4. An interesting problem of chain statistics is to compute the probability of ring closure. This problem is important, for it arises in the closing of DNA circles. Use the FJC model to calculate $<h^2>$ for λ DNA. Assume that for one end of the DNA to be linked to the other, the chain end must lie within a sphere of radius of 10 Å of the first link. What is the probability of this event, $P(h < 10$ Å$)$?

5. Imagine a hypothetical experiment in which you have a polymer chain attached to a wall, and you have managed to get hold of the other end to stretch the molecule. It can be shown that the average extension of a freely jointed chain $<x>$ resulting from such experiment is

$$<x> = L[\coth(Fb/k_BT) - k_BT/Fb],$$

where L is the chain length, F is the pulling force, b the statistical segment describing the chain, k_B the Boltzmann constant and T the absolute temperature. Derive a simpler expression valid in the limit of very small extensions. Using this expression, determine the work done on the chain when it is extended from 1% to 3% of its contour length. What is the change in entropy experienced by the chain?

6. Derive an expression for the mean square end-to-end distance of a worm-like chain (WLC) polymer molecule of length L, possessing two segments: a segment of length l with persistence length P_1 and a segment of $L - l$ of persistence length P_2. (There is no free joint between the segments).