

Molecular Biophysics: Physics 177. Spring 2008. Homework # 3

Helix-coil Transitions & Polyelectrolyte Theory

Assigned February 21. Due February 29 to Birge 225.

1. Using the zipper model, calculate the macroscopic equilibrium constants for the following reactions for a chain of 100 units (each of which can be helix or coil):

$$50\% \text{ helix} \leftrightarrow 20\% \text{ helix} \qquad K_1 = (20\% \text{ helix}) / (50\% \text{ helix})$$

$$75\% \text{ helix} \leftrightarrow 25\% \text{ helix} \qquad K_2 = (25\% \text{ helix}) / (75\% \text{ helix})$$

In your calculation, assume $s = 1$ and $\sigma = 10^{-4}$. [Cantor and Schimmel, Part III, p. 1072]

2. Assume that a chain molecule can exist in three conformations: helix 1, helix 2, and coil. The individual transitions helix 1 \leftrightarrow coil and helix 2 \leftrightarrow coil are highly cooperative and can be described in terms of the zipper model. Let σ and s be statistical weights applicable to the helix 1 \leftrightarrow coil transition, and σ' and s' those applicable to the helix 2 \leftrightarrow coil transition. Calculate the value of σ' , given that the difference in free energy between helix 1 and helix 2 is zero, that $s/s' = 10^{-0.02}$, and that $\sigma = 10^{-4}$. Assume that the chain has 100 units, each of which is capable of being in a helical or coil state. [Cantor and Schimmel, Part III, p. 1072]
3. Apply the zipper model to a DNA circle. Calculate the partition function Z and the fraction Θ of base-paired monomers. Which is greater, $\Theta(\text{circle})$ or $\Theta(\text{linear})$? Why? Under what conditions do they approach the same value? Repeat for the Zimm & Bragg (matrix) model. (Put all results in terms of λ_1 , λ_2 , s , σ , and N).
4. (a) Use the Manning model to find an expression for the density of each component of the ion atmosphere around a line charge as a function of radius r , for a solution containing monovalent salt with concentration c .
(b) Now apply your result to a 100 mM aqueous NaCl solution containing 10 pM of M13 DNA. What are the concentrations of Na^+ and Cl^- at $r = 5$ nm, 10 nm, and 20 nm?
5. Find a journal article on biochemistry or biophysics that uses the Debye-Hückel model. Analyze whether the use of this model is justified under the circumstances. If so, think of some variation on the experimental conditions that would make it unjustifiable. Use your creativity and be quantitative! Minimum ~200 words. To search for articles, I recommend <http://highwire.stanford.edu>. Please attach a photocopy or printout of the article.