Problem set 5
(Hand in by June 3)

Problem 1

Force-extension relationship for the 1D freely-jointed chain. In class, we derived the extension response of a 3D freely-jointed chain to an external force f. In this problem, you will carry out a similar derivation, for the simpler, one-dimensional case. Consider a chain of N stiff segments of length b that always lie along the z-axis. There is a two-state variable σ that takes on the value $\sigma_i = +1$ for each segment that points "forward" in the z-direction, along the external applied force, or $\sigma_i = -1$ for segments that point "backwards", against the external force. The total extension is then given by

$$z = b \cdot \sum_{i=1}^{N} \sigma_i \tag{1}$$

Derive an expression for the average extension $\langle z \rangle$ as a function of N, b, f, and $k_B T$. Hint: You probably want to first write out the partition function Z. Using the partition function, you can write an expression for the ensemble average $\langle z \rangle$, which you can simplify using the "logarithm trick" used in class and familiar from stat mech courses.

Problem 2

Denaturing torque and energy per base pair. In class, we discussed that we can break DNA base pairs by unwinding the helix; the "denaturing torque" for DNA is ≈ -11 pN·nm (the minus sign simply indicates that the helix is untwisted). From this information, obtain a rough estimate of the energy per base pair. Calculate the energy done by untwisting one full turn of the helix by one turn against the melting torque (hint: you need to work in radians) and the corresponding energy per base pair (recall that for DNA, there are 10.5 bp per turn of the helix). Compare this rough estimate of the energy per base pair with the binding energy of a weak (A-T; this is where the helix breaks first) base pair.

Problem 3

Elastic theory of a semiflexible rod. The bending modulus A_{bend} of a semi-flexibel rod is defined by the elastic energy per length dE_{bend}/ds associated with curvature $1/R$ by bending (into an arc of radius R):

$$dE_{bend} = \frac{1}{2} \frac{A_{bend}}{R^2(s)} ds \tag{2}$$

One way to introduce the persistence length L_p is to consider the characteristic length along the rod over which orientational correlation is lost. The orientational correlation is given by the tangent-tangent correlation function:

$$Corr(s) = \langle t(\vec{0}) \cdot t(\vec{s}) \rangle = \langle \cos(\theta(s)) \rangle = \exp(-s/L_p) \tag{3}$$

Show that $k_B T \cdot L_p = A_{bend}$ by

a) Computing the energy required to bend a rod of length s by an arc $\theta = s/R$ of a circle.

b) Expanding $Corr(s)$ to second order of $\theta(s)$ (i.e. considering the $s \ll L_p$ limit).

c) Compute the average $\langle \theta^2(s) \rangle$ over all three-dimensional orientations of the tangent vector at s with the Boltzmann weight of the elastic bending energy. (Note: the simplest approach is to calculate the partition function Z first).