Problem set 6
(Discussion on June 17)

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

DNA overstretching transition. Single-molecule stretching experiments in the 1990s revealed that DNA undergoes an overstretching transition if subjected to forces of $\approx$ 65 pN (Cluzel, *et al.*, *Science* 1996; Smith, *et al.*, *Science* 1996), where it lengthens about 1.7-fold compared to its B-DNA structure. A long-standing debate ensued about what exactly happens upon overstretching. The two possibilities usually considered are DNA melting (i.e. conversion of the double-stranded DNA to two single strands) and conversion of DNA to a double-stranded, but extended and underwound configuration called "S-DNA" ("S" for "stretched"). Van Mameren, *et al.*, *PNAS* 2009, investigated this question using a combination of optical tweezers force-spectroscopy and fluorescence imaging (Available online at `http://www.pnas.org/content/106/43/18231.full.pdf`).

a) What do van Mameren, *et al.* conclude about what happens during the overstretching transition, in terms of S-DNA vs. melting?

b) What evidence do they provide for their conclusion?

c) If we assume that overstretching could involve *both* the formation of S-DNA and DNA melting, how conclusive is their evidence? In particular, does their work rule out the formation of S-DNA upon overstretching?

Problem 3

FJC, revisted. Here we will explicitly derive some identities involving the radius of gyration R_g, which is a very useful measure for the size of a polymer in solution. We assume an ideal FJC (without self-avoidance) with N identical segments of length a. The vectors $\vec{r_i}$ point to segment i. One definition of the radius of gyration is

$$R_g^2 = \frac{1}{N}\sum_{i=1}^{N}\langle(\vec{r_i} - \vec{r}_{mean})^2\rangle \tag{2}$$

Where $\langle ... \rangle$ denotes the statistical average and $\vec{r}_{mean}$ the center of mass position:

$$\vec{r}_{mean} = \frac{1}{N}\sum_{i=1}^{N}\vec{r_i} \tag{3}$$

a) Show that the R_g can also be expressed as

$$R_g^2 = \frac{1}{2N^2}\sum_{i,j=1}^{N}\langle(\vec{r_i} - \vec{r_j})^2\rangle \tag{4}$$

b) Use the fact that for a FJC

$$\langle(\vec{r_i} - \vec{r_j})^2\rangle = |i - j|a^2 \tag{5}$$

($|...|$ denotes the absolute value; note that this identity gives the end-to-end distance result for $i = 0$ and $j = N$) to show that for the FJC

$$R_g^2 = \frac{1}{6}Na^2 \tag{6}$$

Hints: Turn the two summations into two integrals, starting from zero. Adjust the integral limits of the inner integral such that the absolute value is taken into account.