Solution to problem set 5

Problem 1

Force-extension relationship for the 1D freely-jointed chain. We consider the 1D FJC model, with 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

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

To derive an expression for the average extension $\langle z \rangle$, we take the ensemble average, averaging over "states of the world" j, weighting the value that z takes on in each state, z_j by the probability of the state to occur p_j:

$$\langle z \rangle = \sum_j p_j \cdot z_j = \sum_{\sigma_1=\pm 1} ... \sum_{\sigma_N=\pm 1} p(\sigma_1, ..., \sigma_N) \cdot z \tag{2}$$

The probability for a state with energy E_j to occur is given by its Boltzmann factor, properly normalized:

$$p_j = p(\sigma_1, ..., \sigma_N) = \frac{e^{-E_j/(k_B T)}}{Z} = \frac{e^{-(-f \cdot z)/(k_B T)}}{Z} = \frac{e^{(f \cdot b \cdot \sum_{i=1}^{N} \sigma_i)/(k_B T)}}{Z} \tag{3}$$

where the normalization Z is the partition function (i.e. the sum over all Boltzmann factors) and we have used the expression for the extension z from Equation 1.
Inserting the expression for the probabilities and for the length z into Equation 2, we get

$$\langle z \rangle = \sum_{\sigma_1=\pm 1} ... \sum_{\sigma_N=\pm 1} \left(\frac{e^{(f \cdot b \cdot \sum_{i=1}^{N} \sigma_i)/(k_B T)}}{Z} \right) \cdot \left(b \cdot \sum_{i=1}^{N} \sigma_i \right) \tag{4}$$

which can be written short hand by using the "logarithm trick" (you can verify this by simply doing the derivative):

$$\langle z \rangle = k_B T \frac{\partial}{\partial f} \ln \left(\sum_{\sigma_1=\pm 1} ... \sum_{\sigma_N=\pm 1} e^{(f \cdot b \cdot \sum_{i=1}^{N} \sigma_i)/(k_B T)} \right) \tag{5}$$

We notice that the argument of the logarithm is just the product of N independent and identical factors:

$$\langle z \rangle = k_B T \frac{\partial}{\partial f} \ln \left(\left(\sum_{\sigma_1=\pm 1} e^{(f \cdot b \cdot \sigma_1)/(k_B T)} \right) \cdot ... \cdot \left(\sum_{\sigma_N=\pm 1} e^{(f \cdot b \cdot \sigma_N)/(k_B T)} \right) \right) \tag{6}$$

This allows us to write it as a simply product and "pull down" the factor N:

$$\langle z\rangle = k_B T \frac{\partial}{\partial f} \ln \left(e^{(f\cdot b)/(k_B T)} + e^{(-f\cdot b)/(k_B T)}\right)^N = k_B T N \frac{\partial}{\partial f} \ln \left(e^{(f\cdot b)/(k_B T)} + e^{(-f\cdot b)/(k_B T)}\right) \tag{7}$$

Finally, we carry out the derivative with respect to f; to make the results look "pretty", we can additionally use a trigonometric identity:

$$\langle z\rangle = N \cdot b \frac{e^{(f\cdot b)/(k_B T)} - e^{(-f\cdot b)/(k_B T)}}{e^{(f\cdot b)/(k_B T)} + e^{(-f\cdot b)/(k_B T)}} = N \cdot b \cdot \tanh(f \cdot b / k_B T) \tag{8}$$

Problem 2

Denaturing torque and energy per base pair. The denaturing torque Γ_d does work equal to $W = \Gamma_d \cdot \Delta\theta = 11$ pN·nm $2\pi \approx 70$ pN·nm. Divided over 10.5 base pairs, this corresponds to an energy per base pair of ≈ 6.5 pN·nm ≈ 1.5 $k_B T$. This is close to typical base pair energies for AT base pairs, which are in the range of ≈ 2 $k_B T$.

Problem 3

Elastic theory of a semiflexible rod. The connection between the bending modulus of a semi-flexibel and the correlation length over which orientational fluctuations decay is taking from Chapter 10 of Rob Phillips, *et al.*, *Physical Biology of the Cell.* See the separate file for a scan of the corresponding pages.