Homework 5

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■ Problem 1 (10 pnts)

To calculate the corner frequency ω_c and the mean squared fluctuations, $\langle x^2 \rangle^{1/2}$, we must first calculate the stiffness of the DNA from the worm-like-chain expression

$$F = \frac{k_B T}{P} \left(\frac{1}{4(1-x/L)^2} + x/L - \frac{1}{4} \right)$$

For small changes in the extension around some equilibrium extension, x_0, then we can treat the DNA as a spring with stiffness, $\kappa_{\text{DNA}} = \frac{\partial F}{\partial x} |_{x_0}$. Taking the derivative, we find that

$$\kappa_{\text{DNA}} = \frac{\partial F}{\partial x} = \frac{k_B T}{P L} \left(1 + \frac{1}{2(1-x/L)^3} \right)$$

Now the corner frequency in an optical trap is

$$\omega_c = 2 \pi f_c = \frac{\kappa_T}{\gamma}$$

where $\gamma = 6 \pi \eta a$ is the drag coefficient of the bead and κ_T is the total stiffness of the system. a is the radius of the bead and η is the viscosity of the solution.

The total stiffness of the system, since the DNA and the trap act as springs in parallel, is simply the sum of the two stiffnesses

$$\kappa_T = \kappa_{\text{DNA}} + \kappa$$

Thus, the final expression for the corner frequency is

$$\omega_c = \frac{\kappa_{\text{DNA}} + \kappa}{6 \pi \eta r} = \frac{\kappa}{6 \pi \eta a} + \frac{k_B T}{P L} \frac{1}{6 \pi \eta a} \left(1 + \frac{1}{2(1-x/L)^3} \right)$$

By the equipartition theorem,

$$\frac{1}{2} \kappa_T \langle x^2 \rangle = \frac{1}{2} k_B T$$

Thus,

$$\langle x^2 \rangle^{1/2} = \sqrt{\frac{k_B T}{\kappa_T}} = (k_B T)^{1/2} \left(\kappa + \frac{k_B T}{P L} \left(1 + \frac{1}{2(1-x/L)^3} \right) \right)^{-1/2}$$

■ Problem 2 (10 pnts)

■ Part a (2 pnts)

The torque on a magnetic moment in an external magnetic field is

$\tau = \mathbf{M}\times\mathbf{H} = |\mathrm{M}||\mathrm{H}|\sin(\theta)$

■ Part b (2 pnts)

The viscous torque on a sphere with radius a rotating with angular velocity ω is

$\tau = 8\pi\eta a^3 \omega$

■ Part c (2 pnts)

Notice that the torque on the particle is maximum when the particle is rotated at an angle of 45 degrees from the external field, in which case $\sin(90) = 1$

The maximum frequency that the bead will rotate with the magnetic field is the frequency at which the drag torque is equal to this maximum torque.

Setting the two expressions above equal yields

$8\pi\eta a^3 \omega_{\max} = |M||H|\ 1$

$\omega_{\max} = \frac{M H}{8\pi\eta a^3}$

■ Part d (4 pnts)

The torsional persistence length of DNA P_T is related to its torsional stiffness by $P_T = \frac{C}{k_B T}$, and the torque on a piece of DNA of length $L$is given by $\tau = C/L\theta$. Thus, in terms of the torsional persistence length the torque needed to twist a piece of DNA through an angle of θ is $\tau = P_T k_B T/L\theta$. This implies that the torsional stiffness of the DNA is $\kappa_\tau = P_T k_B T/L$.

Now the magnetic field has an effective stiffness as well $d\tau/d\theta = M H \mathrm{Cos}[\theta]$, which if we expand to lowest order in θ yields an effective stiffness of the magnetic field of $\kappa_M = M H$.

These two torsional stiffness add since the torsional springs are in parallel in direct analogy to the linear springs in problem 1. Thus the total effective stiffness of this system is

$k_T = P_T k_B T/L + M H$

and the rms fluctuations in angle are

$$\langle \Delta\theta^2 \rangle = \frac{k_B T}{\kappa_T} = \frac{k_B T}{P_T k_B T / L + M H}$$

■ Problem 3 (6 pnts)

■ Part a (2 pnts)

If the DNA between bead 1 and the second bead is length L (before we add the nick and the third small bead), then if the total angle that the molecules has been twisted is ϕ the torque on this portion of the DNA will be

$$\tau = \frac{C}{L} \phi$$

■ Part b (4 pnts)

Now, since the DNA has been nicked the only portion that can hold torque is the portion between the small third bead and bead 1. Assuming this length between these two beads is L_1, then the torque due to a number of turns N is

$$\tau_N = \frac{C}{L_1} N 2 \pi$$

The rotational drag coefficient for a bead spinning around an axis tangential to its surface is $\gamma_R = 14 \pi \eta R^3$. Thus the viscous torque is

$$\tau_D = 14 \pi \eta R^3 \omega$$

where ω is the angular velocity of the bead. Setting these expressions equal since there are no other torques that are non-zero on average (the Brownian torque averages to zero) yields the final expression for ω

$$\omega = \frac{C}{L_1} \frac{N}{7 \eta R^3}$$

■ Problem 4 (6 pnts)

From previous work we know that the change in free energy upon stretching a DNA molecule slowly is equal to the work done in stretching that molecule. Moreover, the change in free energy is entirely due to a change in entropy. Thus, we have that

$$\Delta \mathrm{S} = -\frac{\Delta \mathrm{G}}{T} = \frac{W}{T} = \frac{1}{T} \int F \, \mathrm{dx}$$

Integrating the relationship between the force and extension for the worm like chain,

$$\int F \, \mathrm{dx} = \frac{k_B T}{P} \int \left(\frac{1}{4 (1 - x/L)^2} + \frac{x}{L} - \frac{1}{4} \right) \mathrm{dx} = k_B T \frac{L}{P} \left(\frac{1}{4 (1 - x/L)} + \frac{x^2}{2 L^2} - \frac{1}{4} \frac{x}{L} \right)$$

Evaluating this integral at the bounds $x = 1/3\, L$ and $x = 2/3\, L$yields

$$W = L\left(\frac{1}{4 (1 - 2/3)} + \frac{1}{2} \left(\frac{2}{3}\right)^2 - \frac{1}{4} \frac{2}{3} \right) - L\left(\frac{1}{4 (1 - 1/3)} + \frac{1}{2} \left(\frac{1}{3}\right)^2 - \frac{1}{4} \frac{1}{3} \right) = \frac{11}{24} \frac{L}{P} k_B T$$

Thus the change in entropy is

$$\Delta S = -\frac{11}{24}\,\frac{L}{P}\,k_B = -0.458\,\frac{L}{P}\,k_B$$