Problem #1: Probability of Conformational States

(a) Consider a protein that can exist in 2 configurations A and B as shown in the figure below. In class we mentioned that the ratio of the probability of being in state B to state A is given by \( P(B)/P(A) = \exp(-\Delta G/kT) \), where \( \Delta G = G_B - G_A \). Derive this relationship. (hint: start with thinking about discrete states where \( P_i = 1/Z \exp(-U_i/kT) \).

![Energy vs. Internal Energy](image)

Problem #2: Biopolymer Mechanics

Recently Maier and Radler (PRL (82) 1911, 1999) have adsorbed DNA onto a lipid bilayer as shown in the figure below. The bilayer is mobile and so we can think about this system as a polymer in 2 dimensions (2-D). Suppose we try to pull on the chain with a given force to get it to 80% of the complete extension, will this require more or less...
force in 2-D compared to 3-D? Why? What is the ratio of the magnitude of the forces (note you can use the large extension limits of the force/extension relationships)?

Problem #3: Stiff Filaments and Cantilevered Beams

Recall that the beam equation for a thin elastic rod is $M = E \frac{I}{R}$ where $M$ is the bending moment, $E$ is the Young’s modulus, $I$ is the second moment of inertia and $\frac{1}{R}$ is the radius of curvature. Now consider the cantilevered beam as shown in the figure below.

Another way to write the beam equation is to consider the tangent angle $\theta(s)$ for a beam in the x-y plane as shown below.

a) Show that if the tangent angle is small then the beam equation can be written as:

$$\frac{d^2y}{dx^2} = \frac{M(x)}{EI}$$
b) Solve (1) for the cantilevered beam shown above.

c) Look at the form of the solution for the free end (y=L). What is the effective spring force constant for this system?

d) What magnitude of forces can you expect to measure with a glass rod of 0.25 µm diameter, length of 100 µm and E=70 GPa.

e) Consider a thermally fluctuating microtubule which is 100 microns long and a persistence length of 60,000 µm. Calculate \( <y(L)^2> \) assuming the chain forms a smooth bend. Do you expect to be able to see measure this using fluorescence microscopy (hint: resolution ~1/wavelength of light)?

Problem #4: Microscopic Description of Diffusion

Consider a small particle in a solution which is fluctuating due to thermal motion. For simplicity we will assume the particle is moving in 1 dimension. The system is described by a location \( x(t) \) at time \( t \), a liquid viscosity \( \mu \) and mass \( m \). The particle is continually colliding with the solvent molecules which impart a random force. A force balance on the particle gives the Langevin equation

\[
m \frac{d^2x}{dy^2} + \xi \frac{dx}{dt} = F(t)
\]

where \( \xi \) is the drag coefficient for the particle in the solvent (6πμa for a sphere of radius a) and \( F \) is a random force with zero mean, i.e. \( <F>=0 \)

a) Multiply the Langevin equation by \( x \) and average the result. And solve the resulting equation to show for \( <x \frac{dx}{dt}> \) to show that \( <x \frac{dx}{dt}> = C \exp(-\gamma t) + \frac{kT}{\xi} \), where \( C \) is a constant of integration and \( \gamma = \xi/m \) is related to the characteristic time of the system.

Hint: you will need to use the equipartition theorem which states that

\[
\frac{1}{2} m <\left( \frac{dx}{dt} \right)^2> = \frac{1}{2} kT. 
\]

Evaluate the constant of integration by assuming that the particle started at the origin.

b) Realizing that \( <x \frac{dx}{dt}> = \frac{d}{dt} <x^2> \), integrte the result from (a) above to derive an expression for the mean-squared displacement \( <x^2> \).

c) Now consider two limiting cases, corresponding to \( t << \gamma^{-1} \) and \( t >> \gamma^{-1} \), i.e. for times that are very short and vary long compared to the characteristic time \( \gamma^{-1} \). Comment on these limiting forms.