Assignment 7
Biophys 4322/5322

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1 Problem 1) Phillips 11.5

Graduate students are smart. They'll figure it out.

2 Problem 2) Phillips 11.6

I'm going to break this up.

2.1 Part a)

Plug $u(x) = Ae^{x/x_0}$ for the deformation induced by the membrane protein into the free energy from hydrophobic mismatch between a membrane protein and the surrounding lipids.

The free energy per unit length is

$$G_h' = \frac{K_b}{2}\int_{R=0}^{\infty}\left(\frac{d^2u}{dx^2}\right)^2 dx + \frac{K_t}{2w_0^2}\int_{R=0}^{\infty} u^2 dx \tag{1}$$

$$= \frac{K_b}{2}\int_0^{\infty}\left(\frac{Ae^{x/x_0}}{x_0^2}\right)^2 dx + \frac{K_t}{2w_0^2}\int_0^{\infty}\left(Ae^{x/x_0}\right)^2 dx$$

$$= \frac{K_b}{2}\frac{A^2}{x_0^4}\int_0^{\infty} e^{2x/x_0}dx + \frac{K_t}{2w_0^2}A^2\int_0^{\infty} e^{2x/x_0}dx$$

$$= \frac{K_b}{2}\frac{A^2}{x_0^4}\left[\frac{x_0}{2}\right] + \frac{K_t}{2w_0^2}A^2\left[\frac{x_0}{2}\right]$$

$$= \frac{K_b A^2}{4x_0^3} + \frac{K_t A^2 x_0}{4w_0^2}. \tag{2}$$

2.2 Part b)

Determine A if $_0$ is the protein-lipid interface. This is silly. At the interface plane $x = 0$ the deformation is

$$u_0 \equiv u(0) = Ae^0 = A. \tag{3}$$

That's all.

So the free energy is

$$G_h' = \frac{K_b u_0^2}{4x_0^3} + \frac{K_t u_0^2 x_0}{4w_0^2}. \tag{4}$$

2.3 Part c)

Minimize the free energy to find the constant x_0.

Do it:

$$\begin{aligned}
\frac{\partial G'_h}{\partial x_0} &= 0 \\
&= \frac{\partial}{\partial x_0}\left[\frac{K_b u_0^2}{4x_0^3} + \frac{K_t u_0^2 x_0}{4w_0^2}\right] \\
&= -\frac{3K_b u_0^2}{4x_0^4} + \frac{K_t u_0^2}{4w_0^2} \\
\frac{4x_0^4}{3K_b u_0^2} &= \frac{4w_0^2}{K_t u_0^2} \\
x_0^4 &= 3w_0^2 \frac{K_b}{K_t} \\
x_0 &= \left(3w_0^2 \frac{K_b}{K_t}\right)^{1/4}. \qquad (5)
\end{aligned}$$

This means we can write G'_h without x_0 as

$$\begin{aligned}
G'_h &= \frac{K_b u_0^2}{4x_0^3} + \frac{K_t u_0^2 x_0}{4w_0^2} \\
&= \frac{u_0^2}{4}\left[\frac{K_b}{x_0^3} + \frac{K_t x_0}{w_0^2}\right] = \frac{u_0^2}{4}\left[\frac{w_0^2 K_b + K_t x_0^4}{w_0^2 x_0^3}\right] \\
&= \frac{u_0^2}{4}\left[\frac{w_0^2 K_b + K_t \left(3w_0^2 \frac{K_b}{K_t}\right)}{w_0^2 x_0^3}\right] \\
&= \frac{u_0^2}{4}\left[\frac{K_b + 3K_b}{x_0^3}\right] = u_0^2\left[\frac{K_b}{x_0^3}\right] \\
&= u_0^2\left[\frac{K_b}{\left(3w_0^2 \frac{K_b}{K_t}\right)^{3/4}}\right] = u_0^2\left(\frac{K_b^{4/3} K_t}{3w_0^2 K_b}\right)^{3/4} \\
&= u_0^2 \frac{1}{3^{3/4}}\left(\frac{K_b K_t^3}{w_0^6}\right)^{1/4} \\
&= \frac{\mathcal{K}}{2} u_0^2 \qquad (6)
\end{aligned}$$

where we have worked hard to define a spring constant

$$\mathcal{K} = \frac{2}{3^{3/4}}\left(\frac{K_b K_t^3}{w_0^6}\right)^{1/4} \qquad (7)$$

Just like in the textbook. Notice the form is exactly the same with only a coefficient of order 1 difference.

2.4 Part d)

Compute the total free energy.

This part and **Part e)** are exactly the same as pg. 449 of the textbook but with our $\mathcal{K}$ (Eq. (7)) instead of Phillips'. The total free energy has three parts

- An undetermined constant G_0
- The energy per unit length G'_h times the circumference $2\pi R$
- The load $\tau \pi R^2$.

So the free energy is

$$
\begin{aligned}
G_{\text{MscL}} &= G_0 + G_h + G_\tau \\
&= G_0 + G'_h 2\pi R - \tau\pi R^2 = G_0 + \mathcal{K} u_0^2 \pi R - \tau\pi R^2 \\
&= G_0 + \frac{2}{3^{3/4}} \left(\frac{K_b K_t^3}{w_0^6} \right)^{1/4} u_0^2 \pi R - \tau\pi R^2
\end{aligned} \tag{8}
$$

2.5 Part e)

What is the critical tension?

Straight from the textbook

$$
\begin{aligned}
\tau_{\text{crit}} &= \mathcal{K} \frac{u_0^2}{R_c + R_0} \\
&= \frac{2}{3^{3/4}} \left(\frac{K_b K_t^3}{w_0^6} \right)^{1/4} \frac{u_0^2}{R_c + R_0}.
\end{aligned} \tag{9}
$$

2.6 Part f)

Does a different solution work with the boundary conditions?

The solution we are supposed to check now is

$$
u(x) = u_0 \left(1 - \frac{x}{x_0} \right) e^{-x/x_0}. \tag{10}
$$

Check that the slope is zero at $x = 0$:

$$
\begin{aligned}
\left. \frac{\partial u}{\partial x} \right|_{x=0} &= \left. -\frac{u_0 x}{x_0^2} e^{-x/x_0} \right|_{x=0} \\
&= 0.
\end{aligned} \tag{11}
$$

Good.

2.7 Part g)

Find the total free energy for this form.

We do everything exactly the same as we already did and find

$$
G'_h = u_0^2 \left(\frac{K_b}{8x_0^3} + \frac{5}{8} \frac{K_t x_0}{w_0^2} \right) \tag{12}
$$

$$
x_0 = \left(\frac{3K_b w_0^2}{5K_t} \right)^{1/4} \tag{13}
$$

$$
\mathcal{K} = \frac{5}{4} \left(\frac{3}{5} \right)^{1/4} \left(\frac{K_t^3 K_b}{w_0^6} \right)^{1/4}. \tag{14}
$$

Use this effective spring constant to find G_{MscL} and τ_{crit}.

3 Problem 3) Phillips 12.4

3.1 Part a)

Show that the drag coefficient for a sphere of radius R rotating at angular velocity ω is given by $K\eta\omega R^3$, where K is a numerical factor.

Stokes drag is

$$
F_s = K\eta R v. \tag{15}
$$

But we're interested in the bead's resistance to torque not linear force:

$$\begin{aligned}\tau_s &= F_s R = (K\eta R v)\, R = K\eta v R^2 = K\eta\,(\omega R)\, R^2 \\ &= K\eta\omega R^3. \end{aligned} \tag{16}$$

3.2 Part b)

Use the figure in the textbook to estimate K in multiples of π if the torque is constantly $\tau = 33$ pN nm.

Rearranging Eq. (16) to match the axes in the figure

$$\eta\omega = \frac{\tau}{K} R^{-3}. \tag{17}$$

The slope in the figure is approximately

$$\begin{aligned}\text{slope} &\approx \frac{20(\text{rot}/s)\text{cP}}{150\mu\text{m}^{-3}} \\ &= \frac{20 \times 2\pi \times 10^{-3}\text{Pa}}{150\,(10^3\text{nm})^{-3}} \\ &= \frac{40 \times 10^{-3}\,\frac{\text{N}}{\text{m}^2}}{150} 10^9 \text{nm}^3 \pi \\ &= \pi \frac{4}{15} 10^6 \text{N} \frac{\text{nm}^3}{\text{m}^2} \\ &= \pi \frac{4}{15} 10^6 10^{12} \text{pN} \frac{\text{nm}^3}{(10^9\text{nm})^2} \\ &= \pi \frac{4}{15} \text{pNnm}. \end{aligned} \tag{18}$$

So if $\tau = 33$ pN nm, the coefficient (in units of π) must be

$$K = \frac{\tau}{\text{slope}} \approx \frac{33}{\pi \frac{4}{15}} \approx 14\pi. \tag{19}$$

3.3 Part c)

Write an expression for the angular velocity of the small bead in terms of the viscosity, the radius, the constant of torsional stiffness C, and the length and the number of whole extra turns in the DNA molecule, N (where $N = \Delta\phi/2\pi$).

Estimate the angular velocity of a $R = 400$ nm bead if the length of DNA is 14.8 kbp and it has been twisted by 50 extra turns. The torsional stiffness of DNA is approximately 400 pN nm^2 . Express your answer in revolutions per second.

We met torsional stiffness in **Assignment 6**. The torque in terms of torsional stiffness is

$$\begin{aligned}\tau &= C\frac{d\phi}{dz} \\ &= C\frac{\Delta\phi}{L} \\ &= C\frac{N2\pi}{L}. \end{aligned} \tag{20}$$

The driving torque and the viscous resistance torque balance so equating the two we have:

$$\begin{aligned}\tau_s &= \tau \\ K\eta\omega R^3 &= C\frac{N2\pi}{L} \\ \omega &= \frac{C}{K}\frac{N2\pi}{\eta L R^3}. \end{aligned} \tag{21}$$

Put in the example numbers and get an example solution:

$$
\begin{aligned}
\omega &= \frac{C}{K}\frac{N2\pi}{\eta LR^3} \\
&\approx \frac{400 \text{ pN nm}^2}{14\pi}\frac{50\times 2\pi}{10^{-3}\text{ Pa s}\,(0.35\times 14.8\times 10^3\text{ nm})\,(400\text{ nm})^3} \\
&= \frac{400\times 100\times 10^3}{14}\frac{\text{pN nm}^2}{\text{Pa s}\,(5000\text{ nm})\,64\times 10^6\text{ nm}^3} \\
&= \frac{4\times 10000\times 10^3}{14\times 64\times 5000\times 10^6}\frac{\text{pN}}{\text{s}\frac{\text{N}}{\text{m}^2}\text{ nm}^2} \\
&= \frac{1}{8\times 14}\times 10^{-3}\frac{\text{pN}}{\text{s}\frac{10^{12}\text{pN}}{10^{18}\text{nm}^2}\text{ nm}^2} \\
&= \frac{1}{112}\times 10^{-3}10^6\frac{1}{\text{s}} \approx 10^{-2}\times 10^3\text{Hz} \\
&= 10Hz = 1.5\text{ rps.}
\end{aligned} \tag{22}
$$

3.4 Part d)

Use these results to determine the rotational drag coefficient of a sphere rotating around its center of mass.

Recall from **Part a)**, the total resistance torque was

$$
\begin{aligned}
\tau_{\text{tot}} &= K\eta\omega R^3 \\
&\approx 14\pi\eta\omega R^3.
\end{aligned} \tag{23}
$$

Part of that is translational (and so uses Stokes drag):

$$
\begin{aligned}
\tau_{\text{trans}} &= F_s R \\
&= (6\pi\eta v R)\,R = 6\pi\eta\,(R\omega)\,R^2 \\
&= 6\pi\eta\omega R^3
\end{aligned} \tag{24}
$$

The difference between the two must be the rotational resistance

$$
\begin{aligned}
\tau_{\text{rot}} &= \tau_{\text{tot}} - \tau_{\text{trans}} = 14\pi\eta\omega R^3 - 6\pi\eta\omega R^2 \\
&= 8\pi\eta\omega R^3
\end{aligned} \tag{25}
$$

4 Problem 4) Phillips 13.2

Derive Eq. 13.32 using more math than is actually necessary.

4.1 Part a)

Take the Fourier transform of the diffusion equation by transforming in the spatial variables to obtain a new differential equation for the concentration in k-space $\widetilde{c}(k,t)$.

The diffusion equation is

$$
\frac{\partial}{\partial t}c(x,t) = D\frac{\partial^2}{\partial x^2}c(x,t). \tag{26}
$$

Take the Fourier transform of both sides to get

$$\begin{aligned}
\left[\widetilde{\frac{\partial c(x,t)}{\partial t}}\right] &= \left[\widetilde{D\frac{\partial^2 c(x,t)}{\partial x^2}}\right] \\
\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{ikx}\left[\frac{\partial c(x,t)}{\partial t}\right]dx &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{ikx}\left[D\frac{\partial^2 c(x,t)}{\partial x^2}\right]dx \\
\frac{\partial}{\partial t}\left[\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{ikx}c(x,t)dx\right] &= \frac{D}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{ikx}\left[\frac{\partial^2 c(x,t)}{\partial x^2}\right]dx \\
\frac{\partial}{\partial t}\widetilde{c}(k,t) &= \frac{D}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{ikx}\left[\frac{\partial^2 c(x,t)}{\partial x^2}\right]dx.
\end{aligned}$$

Nicely done on the LHS but what about the RHS? Answer: Integration by parts. So do it.

$$\begin{aligned}
\frac{\partial}{\partial t}\widetilde{c}(k,t) &= \frac{D}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{ikx}\left[\frac{\partial^2 c(x,t)}{\partial x^2}\right]dx \\
&= \frac{D}{\sqrt{2\pi}}\left[e^{ikx}\frac{\partial c(x,t)}{\partial x}\right]_{-\infty}^{\infty} - \frac{D}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\left[\frac{\partial e^{ikx}}{\partial x}\right]\left[\frac{\partial c(x,t)}{\partial x}\right]dx \\
&= 0 - \frac{D}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\left[ike^{ikx}\right]\left[\frac{\partial c(x,t)}{\partial x}\right]dx
\end{aligned}$$

We have to integrate by parts a second time

$$\begin{aligned}
\frac{\partial}{\partial t}\widetilde{c}(k,t) &= -\frac{Dik}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{ikx}\left[\frac{\partial c(x,t)}{\partial x}\right]dx \\
&= -\frac{Dik}{\sqrt{2\pi}}\left[e^{ikx}c(x,t)\right]_{-\infty}^{\infty} + \frac{Dik}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\left[\frac{\partial e^{ikx}}{\partial x}\right]\left[c(x,t)\right]dx \\
&= 0 + \frac{D\,(ik)^2}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{ikx}c(x,t)dx
\end{aligned}$$

and we recognize that last integral as a Fourier transform so the diffusion equation in Fourier-space is

$$\frac{\partial}{\partial t}\widetilde{c}(k,t) = -k^2 D\widetilde{c}(k,t)$$

4.2 Part b)

Solve the diffusion equation in Fourier-space.

Simple. The solution is

$$\widetilde{c}(k,t) = \widetilde{c}_0 e^{-k^2 D/t}. \tag{27}$$

The thing that takes a touch more work is finding the constant $\widetilde{c}_0$. To do this we take the Fourier transform of the initial condition (that at $t = 0$ the concentration is a delta function $c(x,t) = c_0\delta(x)$)

$$\begin{aligned}
\widetilde{c}_0 = \widetilde{c}(k,0) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{ikx}c(x,0)dx \\
&= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{ikx}c_0\delta(x)dx \\
&= \frac{c_0}{\sqrt{2\pi}},
\end{aligned} \tag{28}$$

which means the concentration in k-space is

$$\widetilde{c}(k,t) = \frac{c_0}{\sqrt{2\pi}}e^{-k^2 D/t}. \tag{29}$$

We do an inverse transform of Eq. (29) to find the concentration distribution in real space

$$\begin{aligned} c(x,t) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx} \widetilde{c}(k,t) dk \\ &= \frac{c_0}{2\pi} \int_{-\infty}^{\infty} e^{-ikx} e^{-k^2 D/t} dk \\ &= \frac{c_0}{2\pi} \sqrt{\frac{\pi}{Dt}} e^{-x^2/4Dt} \\ &= \frac{c_0}{\sqrt{4\pi Dt}} e^{-x^2/4Dt}. \end{aligned} \tag{30}$$

4.3 Part c)

Show that the solution for an arbitrary initial condition $c(x,0)$ can always be written as an integral over the solution for a point source.

Let's do an inverse Fourier transform of the initial conditions in k-space:

$$c(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \widetilde{c}(k,0) e^{-ikx} dk \tag{31}$$

We'll use a mathematical trick by remembering that the Fourier transform of a delta function is

$$\widetilde{\delta(k)} \equiv \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \delta(s-a) e^{-iks} ds = \frac{e^{-ika}}{\sqrt{2\pi}},$$

which means that technically we can say

$$e^{-ika} = \int_{-\infty}^{\infty} \delta(s-a) e^{-iks} ds.$$

Let's substitute the integral of a delta-functions in for the exponent in the arbitrary initial concentration

$$\begin{aligned} c(x,0) &= \frac{\widetilde{c}_0}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \widetilde{c}(k,0) e^{-ikx} dk \\ &= \frac{\widetilde{c}_0}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left[\int_{-\infty}^{\infty} \delta(s-x) e^{-iks} ds \right] \widetilde{c}(k,0) dk \end{aligned} \tag{32}$$

and ta-da we've written the arbitrary distribution as a set of integrals over point sources.

4.4 Part d)

Formally derive $\langle x^2 \rangle = 2Dt$.

Work in real space and use the formal definition of averaging

$$\begin{aligned} \langle x^2 \rangle &= \frac{\int_{-\infty}^{\infty} x^2 c(x,t) dx}{\int_{-\infty}^{\infty} c(x,t) dx} \\ &= \frac{\int_{-\infty}^{\infty} x^2 \frac{c_0}{\sqrt{4\pi Dt}} e^{-x^2/4Dt} dx}{\int_{-\infty}^{\infty} \frac{c_0}{\sqrt{4\pi Dt}} e^{-x^2/4Dt} dx} \\ &= \frac{\int_{-\infty}^{\infty} x^2 e^{-x^2/4Dt} dx}{\int_{-\infty}^{\infty} e^{-x^2/4Dt} dx} = \frac{\int_{-\infty}^{\infty} x^2 e^{-x^2/4Dt} dx}{\sqrt{4\pi Dt}} \\ &= \frac{\frac{\sqrt{\pi}}{2} (4Dt)^{3/2}}{\sqrt{4\pi Dt}} = \frac{1}{2} \frac{(4Dt)^{3/2}}{(4Dt)^{1/2}} \\ &= 2Dt. \end{aligned} \tag{33}$$

5 Problem 5) Phillips 13.5

5.1 Part a)

What are the units of D_r? What is the formula for D_r using the Einstein relation and the rotational friction coefficient?

The rotational diffusion equation is

$$\left\langle \Delta\theta^2 \right\rangle = 2D_r t. \tag{34}$$

Notice that $\Delta\theta^2$ is unitless. Therefore, D_r has units of inverse time.

To find an equation for D_r we use the Einstein relation

$$D_r = \frac{k_\mathrm{B} T}{\gamma} \tag{35}$$

where γ is a friction coefficient (this is worth memorizing or can be found on pg 504). Earlier in the assignment (**Problem 3 Part d)** Eq. (25)), we found that

$$\tau_\mathrm{rot} = 8\pi\eta\omega R^3 = \gamma\omega, \tag{36}$$

where we've identified the rotational friction coefficient $\gamma \equiv 8\pi\eta R^3$ which means that the rotational diffusion coefficient is

$$D_r = \frac{k_\mathrm{B} T}{8\pi\eta R^3}. \tag{37}$$

5.2 Part b)

How long does it take an E. coli to diffuse 1 radian? How far does it swim in that amount of time?

Through the rotational diffusion equation

$$\begin{aligned} t &\sim \frac{\left\langle \Delta\theta^2 \right\rangle}{2D_r} \\ &= \frac{1}{2\left(\frac{k_\mathrm{B} T}{8\pi\eta R^3}\right)} = \frac{4\pi\eta R^3}{k_\mathrm{B} T}. \end{aligned} \tag{38}$$

Assuming room temperature and that the E. coli is a sphere of radius $R \approx 1\mu$m the time is

$$\begin{aligned} t &= \frac{4\pi\eta R^3}{k_\mathrm{B} T} \approx \frac{4\pi \times 10^{-3} Pas 10^{-18} m^3}{4 \times 10^{-21} Nm} \\ &\approx 3s. \end{aligned} \tag{39}$$

If the E. coli swims at a reasonable speed of 20μm/s then it will have travel 60μm or $\times 30$ its "body length" in that amount of time (the R^3 makes it super slow).

6 Problem 6) Phillips 13.7

Graduate students are smart. They'll figure it out.