

PHYSICS 429: Introduction to Biological Physics

May 28 2008

Problem Set 7 These problems are due on Thursday June 5.

1. Nelson 8.7. (a) $v_d = q \frac{\mathcal{E}}{6\pi\eta a}$. We are given $a = 3 \text{ nm}$, $q = 10e$, $\mathcal{E} = 2 \text{ volt cm}^{-1}$. From page 165 $\eta = 9 \times 10^{-4} \approx 10^{-3} \text{ Pa s}$. Thus

$$v_d = \frac{(10e)(200\text{volt/m})}{6\pi(10^{-3}\text{J s m}^{-3})(3 \times 10^{-9} \text{ m})}.$$

Use $1 \text{ eV} = 40 k_B T$ to obtain $v_d = 5.8 \mu\text{ms}^{-1}$.

(b) This time the difference ($\propto 1e$ in velocities enters, since that causes the difference in positions. Thus $\delta x = \delta v \cdot 20 \text{ hours} = \frac{\delta q \mathcal{E}}{6\pi\eta a} (72000) \text{ s} \approx 10 \text{ cm}$. This difference in distance (which is about 1/10 the distance travelled by either ion) is large enough to detect.

2. Nelson 8.8 a,b

a. We generalize the techniques of Sect. 6.1. We use the normalization condition to rewrite the probability of one state in terms of the others as $P_1 = 1 - \sum_{j=2}^N P_j$. Now just as in Sect. 6.1, we separate this term out of the equation for the grand potential, and minimize the grand potential with respect to the independent parameters P_i :

$$\begin{aligned} \Psi_a = & \left(1 - \sum_{j=2}^N P_j \right) (E_1 - \mu N_1) + \left(\sum_{j=2}^N P_j (E_j - \mu N_j) \right) \\ & + k_B T \left[\left(1 - \sum_{j=2}^N P_j \right) \ln \left(1 - \sum_{j=2}^N P_j \right) + \sum_{j=2}^N P_j \ln P_j \right]. \end{aligned}$$

Take the derivative

$$\begin{aligned} \frac{\partial \Psi_a}{\partial P_i} = & 0 = -(E_1 - \mu N_1) + (E_i - \mu N_i) \\ & + k_B T \left[-\ln \left(1 - \sum_{j=2}^N P_j \right) - \left(1 - \sum_{j=2}^N P_j \right) \frac{1}{1 - \sum_{j=2}^N P_j} + \ln P_i + 1 \right] \end{aligned}$$

Exponentiating and recalling $P_1 = 1 - \sum_{j=2}^N P_j$ gives

$$\frac{P_i}{P_j} = \frac{e^{-(E_i - \mu N_i)/k_B T}}{e^{-(E_j - \mu N_j)/k_B T}}.$$

We can lump together all of the factors independent of i to find that $P_i \propto e^{-(E_i - \mu N_i)/k_B T}$ minimizes the free energy. The normalization constant is then $1/\mathcal{Z}$ with $\mathcal{Z} = \sum_{i=1}^N e^{-(E_i - \mu N_i)/k_B T}$ is the grand partition function.

b. Use the probability distribution found in (a) to evaluate the minimum free energy:

$$\begin{aligned} \Psi_a &= \sum_j \left[\frac{e^{-(E_j - \mu N_j)/k_B T} (E_j - \mu N_j)}{\mathcal{Z}} \right] + k_B T \sum_j \left[\frac{e^{-(E_j - \mu N_j)/k_B T}}{\mathcal{Z}} \ln \frac{e^{-(E_j - \mu N_j)/k_B T}}{\mathcal{Z}} \right] \\ &= -k_B T \ln \mathcal{Z}. \end{aligned}$$

3. Nelson C8.11 on page 593. As discussed during lecture, amino acids exist in various protonation states in solution, mainly because they have carboxyl (-COOH) and/or amino (-NH₂) groups. For example, at intermediate pH, glycine has both of these groups charged and is therefore overall neutral.

At low pH, the carboxyl gains a neutralizing proton with $pK=2.35$. At high pH, the amino group loses a proton, becoming neutral, with $pK=9.78$. Find the isoelectric point of glycine, that is, the value of pH at which the average net charge is 0.

Use the law of mass action for the reactions $COOH \rightarrow COO^- + H^+$ and $NH_3^+ \rightarrow NH_2 + H^+$ to obtain

$$\frac{[COO^-][H^+]}{[COOH]} = K_1, \quad \frac{[NH_2][H^+]}{[NH_3^+]} = K_2.$$

At the isoelectric point $[COO^-] = [NH_3^+]$ and $[COOH] = [NH_2]$. Taking the product of the two parts of Eq. (1) gives

$$[H^+]^2 = K_1 K_2.$$

Taking the \log_{10} of both sides of this equation gives $2pH = pK_1 + pK_2$ or $pH = \frac{1}{2}(pK_1 + pK_2) = 0.5(2.35 + 9.78) = 6.065$.

4. Nelson C8.10 on page 592. Reaction-diffusion equation. This is: The discussion of Sect 4.61 explored diffusive transport in a long tube, finding a steady state in which the number density of some dissolved substance, $c(x)$, is a linear function interpolating between the imposed values at the ends of the tubes. In particular, if the two ends are at the same concentration, then $c(x)$ is everywhere constant, there is no net flux, and the steady state is one of equilibrium.

Now suppose that some chemical reaction in the tube removes the dissolved substance. Suppose that each dissolved molecule has a probability to disappear in a time dt equal to $k dt$, where k is a constant. Thus, even if the concentration is spatially uniform (independent of x) near a point x , it will change with time as $\frac{\partial c}{\partial t} = -kc$.

(a) Write an equation for $\frac{\partial c}{\partial t}$ for the case in which c is not spatially uniform. This equation is said to be the reaction-diffusion equation.

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - kc.$$

(b) Again imagine a situation where the concentration is constant in the y and z directions, but is maintained at a fixed value c_0 at both ends of the container, $x = \pm L$. Find the steady-state concentration profile $c(x)$ and the fluxes at each end of the container. Compare with the case of pure diffusion.

In steady state $\frac{\partial c}{\partial t} = 0$, so $D \frac{\partial^2 c}{\partial x^2} = kc$. Solving gives

$$c(x) = Ae^{\alpha x} + Be^{-\alpha x},$$

where $\alpha = \sqrt{k/D}$. The boundary condition is that $c(x = \pm L) = c_0$, so $A = B$ and

$$c(x) = c_0 \frac{\cosh \alpha x}{\cosh \alpha L/2}.$$

The flux is $j = -D \frac{\partial c}{\partial x} = -D\alpha c_0 \tanh \alpha L/2$, $x = L/2$, $= D\alpha c_0 \tanh \alpha L/2$, $x = -L/2$. The non-zero flux is directed inward at each end.

(c) Does the solution you found in (b) correspond to an equilibrium solution? an equilibrium. No, because $j \neq 0$.

5. Nelson C4.20 on page 584.

(a) Suppose that a membrane consists of two types of lipids, A and B . The A lipids assemble in large patches that make up a fraction f of the total membrane area (the rest of the area is composed of

B lipids). Molecule X has a permeability \mathcal{P}_A and \mathcal{P}_B through the two lipids. Find an expression for the permeability \mathcal{P}_{AB} .

$j = -f\mathcal{P}_A\Delta c - (1-f)\mathcal{P}_B\Delta c \equiv -\mathcal{P}_{AB}\Delta c$. Solve for \mathcal{P}_{AB} to get $\mathcal{P}_{AB} = f\mathcal{P}_A + (1-f)\mathcal{P}_B$.

(b) Two membranes A and B have permeabilities \mathcal{P}_A and \mathcal{P}_B . They are joined together to form a single, two-layered membrane. Derive an expression for the permeability of the two-layered membrane, \mathcal{P}_{AB} , in terms of \mathcal{P}_A and \mathcal{P}_B .

We imagine a concentration c_1 outside of the membrane on the A side, a concentration c_3 outside on the B side, and a concentration c_2 between the two membranes. Writing each flux from one region to another, we get $j_{13} = -\mathcal{P}_{AB}(c_1 - c_3)$, $j_{12} = -\mathcal{P}_A(c_1 - c_2)$, $j_{23} = -\mathcal{P}_B(c_2 - c_3)$. All three fluxes are equal because there are no sources or sinks in the membrane. Setting $j_{12} = j_{23}$ gives $\mathcal{P}_A(c_1 - c_2) = \mathcal{P}_B(c_2 - c_3)$ or $c_2 = \frac{\mathcal{P}_A c_1 + \mathcal{P}_B c_3}{\mathcal{P}_A + \mathcal{P}_B}$. Use c_2 in the equation for j_{12} to get an expression for j_{12} in terms of c_1, c_3 . Then set $j_{12} = j_{23}$ to obtain

$$\mathcal{P}_{AB} = \frac{\mathcal{P}_A \mathcal{P}_B}{\mathcal{P}_A + \mathcal{P}_B}.$$

Permeability adds like conductance (inverse resistance) in parallel and series.