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Exercise 10 in FYS381 Biological Physics

Problem 1: Transport of ions through cell membranes

The cell membrane is relatively impermeable to ions. The reason is that the interior of the cell membrane, which mainly consists of the hydrocarbon tails of lipid molecules, is non-polar. Thus it has a low dielectric constant, $\epsilon_m \approx 2\,\epsilon_0$. The surrounding water is, however, highly polarizable and has a large dielectric constant, $\epsilon_w \approx 80\,\epsilon_0$.

For an ion to cross the water-membrane interface it must be wrenched away from the water dipoles. To determine the work needed to jump the interface we can compare the electric self energy for an ion in water with the self energy of an ion inside the membrane.

a) Calculate the difference in electric self-energies for a potassium ion (K^+) with a radius $r = 0.133$ nm. [Hint: You can use the self-energy formula, $E_{self} = q^2/(8\pi\epsilon r)$, for a spherical charge which we derived in the lectures.]

b) What is the relative concentration of potassium ions inside the membrane compared to in the surrounding water?

Problem 2: The Poisson-Boltzmann equation in one spatial dimension

In the lectures we derived the Poisson-Boltzmann equation in one spatial dimension. This equation describes the distribution of monovalent positive counterions ($c(x)$) and the potential ($V(x)$) around a two-dimensional negatively charged macroion. The equation we derived was:

$$\frac{d^2V}{dx^2} = -\frac{ec_0}{\epsilon_w}\,e^{-eV/k_BT} \tag{1}$$

Here c_0 is the (so far unknown) concentration of counterions at the macroion surface defined to be at $x = 0$, and ϵ_w is the dielectric constant of water ($80\epsilon_0$).

In this problem we will go through the mathematical solution of this equation in more detail.

a) Show that by introducing the dimensionless potential $\bar{V}(x) \equiv eV(x)/k_BT$, the Poisson-Boltzmann equation in Eq. (1) can be rewritten as

$$\frac{d^2\bar{V}}{dx^2} = -4\pi l_B c_0\,e^{-\bar{V}} \quad , \tag{2}$$

where the Bjerrum length l_B is defined via

$$l_B \equiv \frac{e^2}{4\pi\epsilon_w k_B T} \quad . \tag{3}$$

b) This equation is non-linear (because the exponential function is non-linear), and for such equations a nice analytical solution is typically hard to find. But here luck is on our side.

Show that the function

$$\bar{V}(x) = B\, ln(1 + (x/x_0)) \tag{4}$$

is a solution to Eq. (2) provided

$$B = 2 \quad \text{and} \quad x_0 = \frac{1}{\sqrt{2\pi l_B c_0}} \quad . \tag{5}$$

c) We have not yet found a unique solution since the parameter c_0 is still undetermined. To specify the unique solution we must use *boundary conditions*. These boundary conditions are

1. The surface form of the Gauss law taken from electromagnetism reads

   $$\varepsilon|_{\text{surface}} = -\left.\frac{dV}{dx}\right|_{\text{surface}} = -\frac{\sigma_q}{\epsilon_w} \tag{6}$$

   where ε is the electric field in the x-direction, and -σ_q is the (negative) uniform charge density at the surface (charge per area).

2. The analogous condition at infinity ($x \to \infty$) is

   $$-\left.\frac{dV}{dx}\right|_{\infty} = 0 \tag{7}$$

   because no charge is located there.

In addition we choose the *convention* that

$$V(0) = 0 \quad . \tag{8}$$

Note that the trial function in Eq. (4) already fulfills the chosen convention in Eq. (8).

I. Show that the boundary condition in Eq. (6) in term of the dimensionless potential $\bar{V}$ can be written as

$$\left.\frac{d\bar{V}}{dx}\right|_{\text{surface}} = 4\pi l_B \frac{\sigma_q}{e} \quad . \tag{9}$$

II. Show that this boundary condition imposes the requirement

$$c_0 = 2\pi l_B \left(\frac{\sigma_q}{e}\right)^2 \tag{10}$$

and that x_0 is thus determined to be

$$x_0 = \frac{e}{2\pi l_B \sigma_q} \quad . \tag{11}$$

III. Show that the boundary condition in Eq. (7) is fulfilled.

d) Find the concentration profile $c(x)$. Calculate the the total density of counterions (total number of counterions per surface area),

$$\int_0^\infty c(x)\, dx \quad , \tag{12}$$

and verify that the whole system is electrically neutral.

e) What would the electrical force on a test particle with charge Q put into this counterion layer be?

Problem 3: Effect of hydrogen bonds on water (problem 7.6 in Nelson)

In the lectures we learned that the average number of H-bonds between a molecule of liquid water and its neighbors is about 3.5. Assume that these bonds are the major interaction holding liquid water together and that each H-bond lowers the energy by about $9k_BT_r$. Using these ideas, find a numerical estimate for the heat of vaporization of water, Q_{vap}. Note that Q_{vap} is the energy per unit volume we must add to liquid water (just below the boiling point) to convert it completely to steam (just above its boiling point). That is, the heat of vaporization is the energy needed to separate every molecule from every other one.
Compare your estimate with the experimental value $Q_{vap} = 2.3 \cdot 10^6$ J/kg.