Physics 480 and 581: Homework #2
Due September 28, 2010

1. (5 points)

   Several amino acid side chains can gain or loose charge. For each of these side chains, calculate the average charge at pH 5.0, 7.0 and 9.0. Use the pKa values found here `http://en.wikipedia.org/wiki/Protein_pKa_calculations`.

2. (5 points)

   Consider the following simple model for a neuron. A long, thin cell of length L contains a source of a particular protein at one end. The source maintains a concentration, c_0 of this protein at the end of the cell. The other end of the cell acts as a perfect sink. Use Fick's first and second equations to find the concentration along the length of the cell as well as the number flux. The cell is one meter long, and small vesicles with radius of $R = 50$ nm are observed moving along neurons with a net velocity of 400 mm per day. Can this be explained by diffusion?

3. (10 points)

   For an isolated, charged, planar surface in solution there does exist an analytical solution for the Poisson-Boltzmann equation (See chapter 7 of Nelson) given by:

   $$\bar{V}(x) = -2\log\frac{1 + e^{-(x+x_*)/\lambda_D}}{1 - e^{-(x+x_*)/\lambda_D}}$$

   where is $\bar{V}(x) = eV/k_BT$ and λ_D is the Debye screening length. If the surface in immersed in solution with an NaCl concentration of 100 mM, at what surface charge density does the Debye-Hueckel solution diverge from the true expressions at distances greater than 0.5 nm? Give some thoughts about when this might occur (if ever) in biology. Plot $c(x)_+$ and $c(x)_-$ at surface charge densities above and below the region where the expressions found using the Debye-Hueckel equation diverges from that found from the Poisson-Boltzmann equation.

4. (581 only: 10 points) For the above problem, use a numerical method to solve the Poisson-Boltzmann equation equation and compare your results to the analytical solution for the condition when the Debye-Hueckel equation is not appropriate. Next, use your approach to solve the Poisson-Boltzmann equation for the case of a charged, spherical shell in salt solution. At 100 mM salt concentration, at what surface charge density does the numerical solution diverge from the linearized solution? Plot your results.