

Reading: You should read Chapter 5.1, 5.2, 5.4, 5.5 (omit 5.5.2, 5.5.3). You can also begin reading Chapter 6.1.1, 6.1.2.

Problem 1: Some Math:

(a) Show that the variance, $var(x) = \sum_i (x_i - \langle x \rangle)^2 P(x_i) = \langle x^2 \rangle - (\langle x \rangle)^2$. In words, the variance is just the average of x^2 minus the square of the average, $\langle x \rangle$.

(b) Average of gaussian distribution. The gaussian distribution is given by

$$P(x) = \frac{1}{\sigma \sqrt{2\pi}} \exp\left(-\frac{(x-x_0)^2}{2\sigma^2}\right)$$

Show that the average of x is x_0 . TIP: You'll need to do a change of variables to make the integral simpler. You will have one integral

that will look like $\int_{-\infty}^{\infty} dy y \exp(-y^2)$. Without doing any integration, convince

yourself and explain why this integral is zero. Show all your steps in doing this calculation.

(c) Variance of gaussian distribution. Show that the variance of the gaussian distribution, $var(x) = \sigma^2$. TIP: to carry out the integration, you will need the following trick

from calculus. The integral $\int dy \exp(-by^2) = \sqrt{\pi/b}$.

- i. Take the derivative with respect to b of the left and right hand sides of the above equation. Does the integral look like the integral that you need to evaluate?
- ii. What is the value of your integral given the above result? (Your integral is the same as in (i) with $b = 1$).

(d) Stirling's formula:

- i. Using the property $\ln(AB) = \ln(A) + \ln(B)$, write $\ln N!$ as a sum of N terms.
- ii. For large N , this sum can be converted into an integral. Evaluate the integral and show that Stirling's formula is the result.

Problem 2: Kinetic Theory:

(a) Why don't the air molecules in a room fall to the floor? To answer this question compare the average kinetic energy of an O_2 molecule at room temperature to its gravitational potential energy if it is at the ceiling of a room which has a height of 3 m. How cold would the room have to get such that the average kinetic energy became equal to the gravitational potential energy, such that the molecules would start falling to the floor?

(b) Why does dirt fall to the floor? To answer this do the same calculation as in (a) except

now for a piece of dirt which you can assume has a mass that is the same as a cube of water which measures $50 \mu m$ on a side.

(c) Using the ideal gas law, show that our result for the root-mean-square (rms) speed can also be written in terms of the pressure, P and density of the gas, ρ via

$$v_{rms} = \sqrt{3P/\rho} .$$

(d) What is the rms speed of a protein of mass 50000 da inside a cell at a temperature of $37^\circ C$?

Problem 3: Potential Energy and Molecular Vibrations

The potential energy of a flexible molecule is given by the equation

$U(x) = x^4 - 2x^2 - 1$ in units of $k_B T$ and where the conformational coordinate of the molecule, x , is in nm.

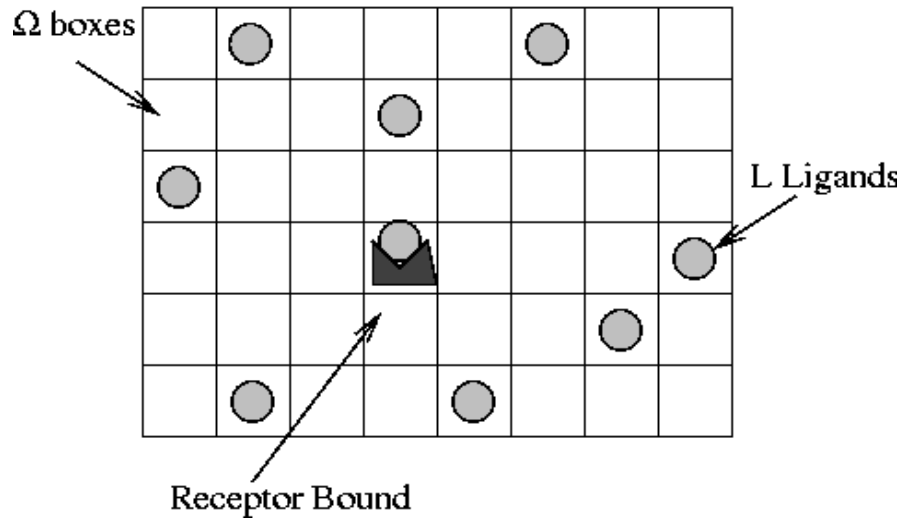
(a) At what value(s) of x is $U(x)$ minimum?

(b) What is the effective spring constant(s) at the minima?

(c) If the molecule has an additional energy $0.5k_B T$ (T is 293 K) above the value at the minima, what will the amplitude of its vibration be at the minima?

Problem 4: Entropy of Ligand Binding:

In this problem you will compute the entropy and free energy of a ligand binding to a receptor. In order to have a simple model for the problem, we will assume that the solution will be treated as a lattice, with ligands occupying various sites on the lattice.



(a) Show that the number of states for no bound ligand and 1 bound ligand are

$$W_0 = \frac{\Omega!}{L!(\Omega-L)!} \quad \text{and} \quad W_1 = \frac{\Omega!}{(L-1)!(\Omega-L+1)!} \quad \text{respectively.}$$

(b) Compute the entropy change between the bound and unbound state. Use the approximation that $\Omega!/(\Omega-L)! \approx \Omega^L$ for large Ω .

(c) Re-express your result in (b) using the concentration of ligand, $c = L/V$ and a reference concentration where all sites are occupied, $c_0 = \Omega/V$ where V is the volume of the box. Show that for a small ligand that takes up a lattice site with volume = 1 nm^3 , that $c_0 = 1.7 \text{ Molar}$.

(d) If in the bound state, the system gains energy, $\epsilon < 0$, what is the free energy change between the bound and unbound states.

(e) For a concentration of ligand, $c = 1 \text{ }\mu\text{M}$, using your value of c_0 above, what value does ϵ need to be so that the probabilities of being in the bound or unbound state are equal?