Exercise 03

1. Mathematics of Curvature

a)

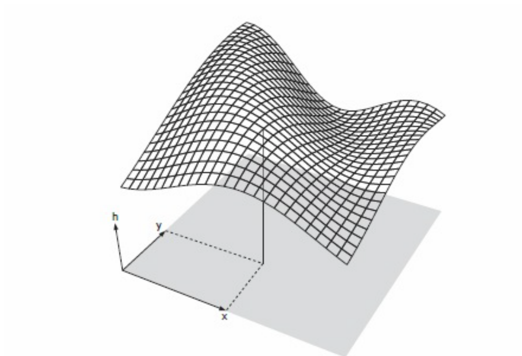

Figure 1: The height function, h(x, y). The surface of the membrane is characterised by a height at each point (x, y). This height function tells us how the membrane is disturbed locally from its preferred flat reference state.

b) The principle radii of curvature are the eigenvalues of the matrix of second derivatives:

$$\begin{pmatrix} \frac{\partial^2 h}{\partial x_1^2} & \frac{\partial^2 h}{\partial x_1 x_2} \\ \frac{\partial^2 h}{\partial x_2 x_1} & \frac{\partial^2 h}{\partial x_2^2} \end{pmatrix} = \begin{pmatrix} 2 & 1 \\ 1 & -4 \end{pmatrix}$$

And the eigenvalues are found by solving

$$det\begin{pmatrix} 2-\kappa & 1 \\ 1 & -4-\kappa \end{pmatrix} = 0$$

which reduces to

$$0 = -(2-\kappa)(4+\kappa) - 1$$
$$0 = \kappa^2 + 2\kappa - 9$$
$$\kappa_{1,2} = \pm\sqrt{10} - 1$$

c) The bending free energy in terms of curvature and bending rigidity K_b is given by

$$G_{bend} = \frac{K_b}{2}\int da(\kappa_1(x,y) + \kappa_2(x,y))^2$$
$$= \frac{K_b}{2}\int da(-\sqrt{10} - 1 + \sqrt{10} - 1)^2$$

$$= 2K_b \int da$$
$$= 2K_b * "surface\ area"$$

The surface area is given by

$$SA = \int_0^1 \int_0^1 \left(\sqrt{\left(\frac{\partial h}{\partial x_1}\right)^2 + \left(\frac{\partial h}{\partial x_2}\right)^2 + 1} \right) dx_1 dx_2$$
$$= \int_0^1 \int_0^1 \left(\sqrt{(2x_1 + x_2)^2 + (x_1 - 4x_2)^2 + 1} \right) dx_1 dx_2$$
$$= \int_0^1 \int_0^1 \left(\sqrt{4x_1^2 + 4x_1x_2 + x_2^2 + x_1^2 - 8x_1x_2 + 16x_2 + 1} \right) dx_1 dx_2$$
$$= \int_0^1 \int_0^1 \left(\sqrt{5x_1^2 - 4x_1x_2 + 17x_2^2 + 1} \right) dx_1 dx_2$$

which has to be integrated numerically and yields 2.6, implying a bending energy of $5.2K_b$.

2. Distinguishable ligands

As illustrated in Fig. 2, L indistinguishable particles distributed across Ω discrete positions can adopt $\frac{\Omega!}{L!(\Omega-L)!}$ distinct configurations. This is the multiplicity of the L free ligands state. However, when those ligands are distinguishable, this result becomes

$$\#\ arrangements = \frac{\Omega!}{(\Omega - L)!}$$

The partition function can then be written as

$$Z = e^{-\beta\epsilon_{sol}} \frac{\Omega!}{(\Omega - L)!} + Le^{-\beta\epsilon_b} \frac{\Omega!}{(\Omega - (L-1))!}$$

where the second term occurs L times because we have L different choices for which a ligand binds the the receptor.
As a result, we can write the probability that the receptor will be bound by a ligand as

$$p_{bound} = \frac{Le^{-\beta\Delta\epsilon} \frac{\Omega!}{(\Omega - (L-1))!}}{\frac{\Omega!}{(\Omega - L)!} + Le^{-\beta\Delta\epsilon} \frac{\Omega!}{(\Omega - (L-1))!}}$$

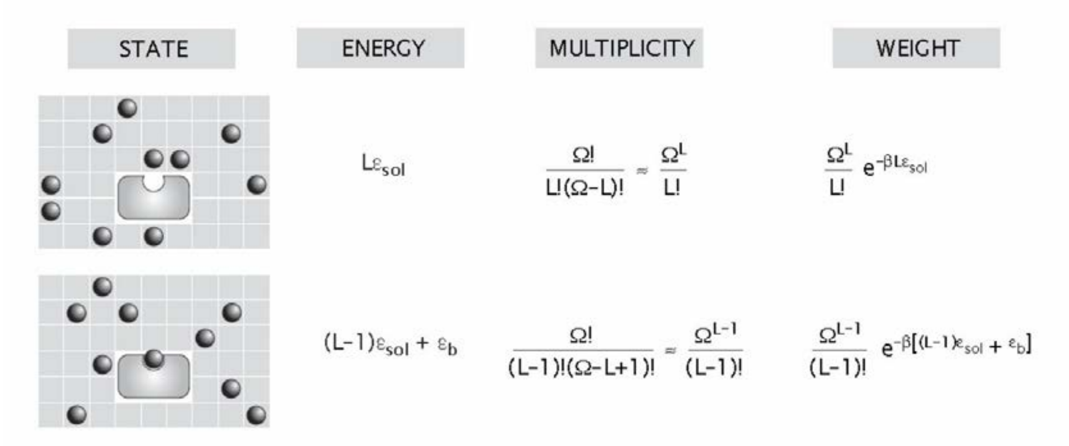

Figure 2: States and weights diagram for ligand-receptor binding. The cartoons show a lattice model of the solution for the case in which there are L ligands. In (A) the receptor is unoccupied. In (B) the receptor is occupied by a ligand and the remaining L-1 ligands are free in solution.

If we invoke our usual approximation

$$\frac{\Omega!}{(\Omega - L)!} \approx \Omega^L$$

this can be simplified to

$$p_{bound} = \frac{L\Omega^{L-1}e^{-\beta\Delta\epsilon}}{\Omega^L + L\Omega^{L-1}e^{-\beta\Delta\epsilon}}$$

Dividing top and bottom by Ω^L results in our usual expression for p_{bound}:

$$p_{bound} = \frac{\frac{L}{\Omega}e^{-\beta\Delta\epsilon}}{1 + \frac{L}{\Omega}e^{-\beta\Delta\epsilon}}$$

This demonstrates the equivalence of the results for the distinguishable and indistinguishable cases.