Physics 187

Homework #4 Solutions

1. Jackson 5.1

Derive: $K_T Y_1 = K_R Y_0$

Using $K_T = \dfrac{[T_1]}{[T_0][L]}$, $K_R = \dfrac{[R_1]}{[R_0][L]}$, $Y_0 = \dfrac{[R_0]}{[T_0]}$

$Y_1 = \dfrac{[R_1]}{[T_1]}$

From these $K_T Y_1 = \dfrac{[T_1]}{[T_0][L]} \cdot \dfrac{[R_1]}{[T_1]} = \dfrac{[R_1]}{[T_0][L]}$

$$K_R Y_0 = \frac{[R_1]}{[R_0][L]} \cdot \frac{[R_0]}{[T_0]} = \frac{[R_1]}{[T_0][L]}$$

So $K_T Y_1 = K_R Y_0$.

3. Use energy balance to express Y_0 / Y_{AB} in terms of the binding constants

A B binding scheme

$$\begin{array}{ccc} T_0 + A & \overset{K_{TA}}{\rightleftharpoons} & T_A \\ Y_0 \downarrow\uparrow & & \downarrow\uparrow Y_A \\ R_0 + A & \rightleftharpoons & R_A \end{array}$$

and the same for B.

To put these together we need a new picture.

$$
\begin{tikzcd}
T_B + A \arrow[r, shift left, "K_{TB}"] \arrow[d, shift left] \arrow[rrr, bend left, "K_{TBA}"] & T_0 + A \arrow[l, shift left] \arrow[r, shift left, "K_{TA}"] \arrow[d, shift left, "Y_0"] & T_A + B \arrow[l, shift left] \arrow[r, shift left, "K_{TAB}"] \arrow[d, shift left, "Y_A"] & T_{AB} \arrow[l, shift left] \arrow[d, shift left, "Y_{AB}"] \\
R_B + A \arrow[u, shift left, "Y_B"] \arrow[r, shift left, "K_{RB}"'] \arrow[rrr, bend right, "K_{RBA}"'] & R_0 + A \arrow[u, shift left] \arrow[l, shift left] \arrow[r, shift left, "K_{RA}"'] & R_A + B \arrow[u, shift left] \arrow[l, shift left] \arrow[r, shift left, "K_{RAB}"'] & R_{AB} \arrow[u, shift left] \arrow[l, shift left]
\end{tikzcd}
$$

Anyway, for our calculation we need to consider two paths

$$RT \log Y_0 + RT \log K_{RA} + RT \log K_{RAB}$$

$$= RT \log K_{TA} + RT \log K_{TAB} + RT \log Y_{AB}$$

$$\Rightarrow \quad Y_0 K_{RA} K_{RAB} = Y_{AB} K_{TA} K_{TAB}$$

$$\boxed{\frac{Y_0}{Y_{AB}} = \frac{K_{TA} K_{TAB}}{K_{RA} K_{RAB}}}$$

4. In the MWC model find the fraction of R-state protein as a function of [L].

$$A = \sum_{i=0}^{n} [R_i] \Big/ \sum_{i=0}^{n} \left([R_i] + [T_i]\right)$$

We already derived (see class notes)

$$\sum_{i=0}^{n} [R_i] = [R_0]\left[1 + K_R [L]\right]^n$$

$$\sum_{i=0}^{n} [T_i] = [T_0]\left[1 + K_T [L]\right]^n$$

$$A = \frac{[R_0]\left(1+K_R[L]\right)^n}{[R_0]\left(1+K_R[L]\right)^n + [T_0]\left(1+K_T[L]\right)^n}$$

or
$$A = \frac{Y_0\left(1+K_R[L]\right)^n}{Y_0\left[1+(K_R[L])\right]^n + \left(1+K_T[L]\right)^n}$$

5. Show that the above result goes to Eq. 5.4 when $n=1$

$$A_{n=1} = \frac{1+K_R[L]}{1+K_R[L]+\frac{1}{Y_0}\left(1+K_T[L]\right)}$$

But $K_T Y_1 = K_R Y_0$

$$A_{n=1} = \frac{1+K_R[L]}{1+K_R[L]+\frac{1}{Y_0}\left(1+\frac{K_R Y_0}{Y_1}[L]\right)}$$

$$= \frac{1+K_R[L]}{(1+Y_0^{-1})+[L]K_R(1+Y_1^{-1})}$$ ← Eq'n 5.4 checks

9. Derive the KNF binding curve for a dimer.

We have  Following the class notes p. 59

$$\frac{[P_1]}{[P_0][L]} = e^{-\Delta G/RT} = 2K_s\sigma$$ ← domain wall

↑ two half-filled states.

$$\frac{[P_2]}{[P_1][L]} = \frac{1}{\sigma}K_s\frac{1}{2}$$ ← lose entropy

↑ remove domain wall

$$[P_1] = [P_0][L]\, 2 K_s \sigma$$

$$[P_2] = \frac{1}{2\sigma} K_s\, [P_1][L] = [P_0][L]^2 K_s^2$$

Binding curve $\Rightarrow$

$$B = \frac{[P_1] + 2[P_2]}{2\left\{[P_0] + [P_1] + [P_2]\right\}}$$

$$B = \frac{[P_0][L]\, 2K_s\sigma + 2[P_0][L]^2 K_s^2}{2\left\{[P_0] + [P_0][L]\, 2K_s\sigma + [P_0][L]^2 K_s^2\right\}}$$

$$B = \frac{K_s\sigma[L] + [L]^2 K_s^2}{1 + 2K_s\sigma[L] + [L]^2 K_s^2}$$

for large σ: $$B \cong \frac{K_s\sigma[L]}{2K_s\sigma[L] + [L]^2 K_s^2}$$

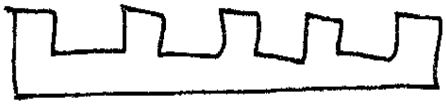
$$\Rightarrow\quad B \cong \frac{1}{2}\,\frac{1}{1 + [L](K_s/2\sigma)}$$

effective binding constant for the second ligand.

for σ large and $[L]$ small.

$K_s\sigma[L] \ll 1$

$$B \cong \frac{K_s\sigma[L]}{1 + 2K_s\sigma[L]}$$

5.  Remember periodic bc.

How many states are there?

			Domain walls
P_0	$\_\ \_\ \_\ \_$	1 way	0
P_1	$\_\ \_\ \_\ \underline{X}$	4 ways	1
P_2	$\_\ \underline{X}\ \_\ \underline{X}$	2 ways	2
P_2'	$\_\ \_\ \underline{X}\ \underline{X}$	4 ways.	1
P_3	$\underline{X}\ \underline{X}\ \underline{X}\ \_$	4 ways	1
P_4	$\underline{X}\ \underline{X}\ \underline{X}\ \underline{X}$	1 way	0.

Total of $2^4 = 16$ states.

$$\frac{[P_1]}{[L][P_0]} = \frac{4}{1} K_s \sigma \qquad \frac{[P_2]}{[L][P_1]} = \frac{2}{4} K_s \sigma$$

and $$\frac{[P_2']}{[L][P_1]} = \frac{4}{4} K_s \qquad \frac{[P_3]}{[L][P_2]} = \frac{4}{2\sigma} K_s$$

$$\frac{[P_4]}{[L][P_3]} = \frac{1}{4\sigma} K_s$$

Solve for all concentrations:

$$[P_1] = 4 K_s \sigma [L][P_0]$$

$$[P_2] = \frac{1}{2} K_s \sigma [L]^2 4 K_s \sigma [P_0] = 2 K_s^2 \sigma^2 [L]^2 [P_0]$$

$$[P_2'] = K_s [L][P_1] = 4 K_s^2 \sigma [L]^2 [P_0]$$

$$[P_3] = \frac{2}{\sigma} K_s [L][P_2] = \frac{2}{\sigma} K_s [L](2 K_s^2 \sigma^{-2} [P_0])[L]^2$$

$$[P_3] = 4 K_s^3 \sigma [P_0][L]^3$$

$$[P_4] = \frac{1}{4\sigma} K_s \, 4K_s^3 \sigma [P_0][L]^3 [L] = K_s^4 [L]^4 [P_0]$$

Binding curve:

$$B = \frac{[P_1] + 2([P_2] + [P_2']) + 3[P_3] + 4[P_4]}{4\{[P_0] + [P_1] + [P_2] + [P_2'] + [P_3] + [P_4]\}}$$

$$B = \frac{4K_s^4 L^4 P_0 + 4K_s \sigma L P_0 + 4K_s^2 \sigma^{-2} L^2 P_0 + 8K_s^2 \sigma L^2 P_0 + 12 K_s^3 \sigma P_0 L^3}{4\{ \qquad \}}$$

$$\boxed{B = \frac{K_s \sigma [L] + K_s^2(\sigma^{-2} + 2\sigma)[L]^2 + 3K_s^3 \sigma [L]^3 + K_s^4 [L]^4}{1 + 4K_s \sigma [L] + 2K_s^2(\sigma^2 + 2\sigma)[L]^2 + 4K_s^3 \sigma [L]^3 + K_s^4 [L]^4}}$$