SM-1 January 2012

N monometers

two states: coil

helix

$T \to$ temperature.

$E_w \to$ binding energy of monomer in coil

$E_m \to$ bindin energy of monomer helix.

$S_w \to$ entropy increase of water per monomer in h.

$S_p \to$ entropy increase of configuration per monomer c.

$$\Delta G_{c \to h} = (N-2)\left[(E_w - E_m) - T\left(S_w - \frac{N}{N-2} S_p\right)\right]$$

a. Determine critical temperature of coil-helix transition.

$P_c = P_h = \frac{1}{2}$

$\Delta G = 0 \to$ system would have no preference between states

$$0 = (N-2)\left[(E_w - E_m) - T_c\left(S_w - \frac{N}{N-2} S_p\right)\right]$$

$$(N-2)(E_w - E_m) = T_c\left[(N-2)S_w - N S_p\right]$$

$$T_c = \frac{(N-2)(E_w - E_m)}{(N-2)S_w - N S_p}$$

b For what values of N do we expect no transition to happen

No transition for $T_c < 0$

$$\frac{(N-2)(E_w - E_m)}{(N-2)S_w - N S_p} < 0$$

$$(N-2)(E_w - E_m) < (N-2)S_w - N S_p$$

$$N(E_w - E_m - S_w + S_p) < 2(E_w - E_m) - 2S_w = 2(E_w - E_m - S_w)$$

$$N < \frac{2(E_w - E_m - S_w)}{E_w - E_m - S_w + S_p}$$

No transition for $N \leq \frac{2(E_w - E_m - S_w)}{E_w - E_m - S_w + S_p}$.

Not sure if N should be a max or a min?

c. Determine sharpness of transition.

$$\left.\frac{dP_h}{dt}\right|_{T=T_C}$$

$$P_h = \frac{e^{-\beta E_m}}{e^{-\beta E_m} + e^{-\beta E_w}}$$

$$\frac{dP_h}{dT} = \frac{d}{dT}\left(e^{-E_m/k_BT}\right)\left(e^{-E_m/k_BT} + e^{-E_w/k_BT}\right)^{-1} = \frac{\left(e^{-E_m/k_BT} \cdot \frac{-E_m}{k_BT^2}\right)}{e^{-E_m\beta} + e^{-E_w\beta}} - \frac{\left[e^{-E_m/k_BT}\left(-\frac{E_m}{k_BT^2}\right) + e^{-E_w/k_BT}\left(-\frac{E_w}{k_BT^2}\right)\right]}{\left(e^{-E_m\beta} + e^{-E_w\beta}\right)^2} e^{-E_m}$$

$$= \frac{-E_m}{k_BT^2}\frac{z\, e^{-E_m\beta}}{z^2} + \frac{E_m e^{-2E_m\beta} + E_w e^{-E_m\beta - E_w\beta}}{k_BT^2 \quad z^2}$$

$$= \frac{-E_m \cdot \left(e^{-2E_m\beta} + e^{-\beta(E_m+E_w)}\right) + E_m e^{-2E_m\beta} + E_w e^{-(E_w+E_m)\beta}}{k_BT^2 \quad z^2}$$

$$= \frac{e^{-\beta(E_m+E_w)}\left(E_w - E_m\right)}{k_BT^2 \quad z^2} \qquad T_c = \frac{(N-2)(E_w - E_m)}{(N-2)S_w - NS_p}$$

For T_c:

$$\frac{e^{-\beta(E_m+E_w)}\left(E_w - E_m\right)}{k_B\, z^2} \quad \frac{((N-2)S_w - NS_p)^2}{(N-2)^2\,(E_w - E_N)^2}$$