# PROTEIN FOLDING

CONSIDER A BETA-HAIRPIN FORMING PEPTIDE AS A SIMPLE LATTICE MODEL:

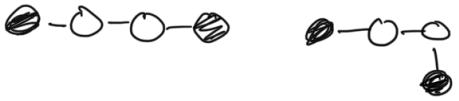
FOLDED

$U = -\varepsilon$

$N_{conf} = 1$

$\varepsilon > 0$

UNFOLDED



$U = 0$

$N = 4$ DISTINCT CONFORMATIONS

(1) WHAT IS THE PROBABILITY $P_{FOLDED}(\beta)$ OF THE FOLDED STATE AS A FUNCTION OF INVERSE TEMPERATURE $\beta = \frac{1}{k_B T}$ ?

(2) WHAT IS THE STABILITY OF THE FOLDED STATE,

$$\Delta F(\beta) = F_{UNFOLDED}(\beta) - F_{FOLDED}(\beta)$$

IN UNITS OF $k_B T$ ?

(3) AS TEMPERATURE $T$ INCREASES, HOW DOES $\Delta F$ CHANGE? DOES IT GET MORE POSITIVE ($\frac{d}{dT}\Delta F > 0$) OR NEGATIVE ($\frac{d}{dT}\Delta F < 0$)?

(4) AT WHAT TEMPERATURE $T_m$ IS THE PROTEIN 50% UNFOLDED ($\Delta F = 0$)?