

Model for Protein Folding. (a.) Since the total energy is the sum of independent contributions from each peptide, the distribution of energies is Gaussian by the central limit theorem. This is the same idea as random walk statistics of a polymer chain. Then the variance is $\kappa^2 = Ne^2$, so $\kappa \sim \sqrt{N}$, just like the end-to-end distance of a polymer chain scales as \sqrt{N} .

(b.) The probability of a single state with energy E is $Q^{-1}e^{-\beta E}$, so the probability of all states with energy E is

$$p(E) = \frac{1}{Q}\Omega(E)e^{-\beta E} = \frac{\Omega(E)e^{-\beta E}}{\int dE\Omega(E)e^{-\beta E}} \quad (1)$$

We talked about this when we showed how the canonical partition function is a Laplace transform of the microcanonical partition function Ω .

(c.) At the folding temperature T_f , $p(-Ne_0) = p(0)$, so in general

$$\frac{p(E)}{p(0)} = \exp\left(-\frac{E^2}{2Ne_0^2} - \frac{E}{kT_f}\right) = 1 \quad (2)$$

so inserting $E = -Ne_0$ which implies

$$\frac{N^2e_0^2}{2Ne_0^2} - \frac{Ne_0}{kT} = 0 \quad (3)$$

so then

$$T_f = \frac{2e_0}{k} \quad (4)$$

(d.) At higher temperatures, the entropy of the system dominates and favors states with larger energies. In the limit of high T , the average energy is $\langle E \rangle_0$ at the peak of the Gaussian, which motivates the comparison required in (c). At lower temperature, the states with lower energy become more important until finally $p(E) \geq p(0)$, or the lowest energy states dominates. This is how the protein “folds” into its native state at low temperatures. While the model is not very realistic, people claim that this simple Gaussian model captures the basic physics of protein folding. Decide for yourself.