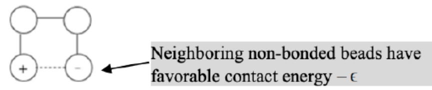
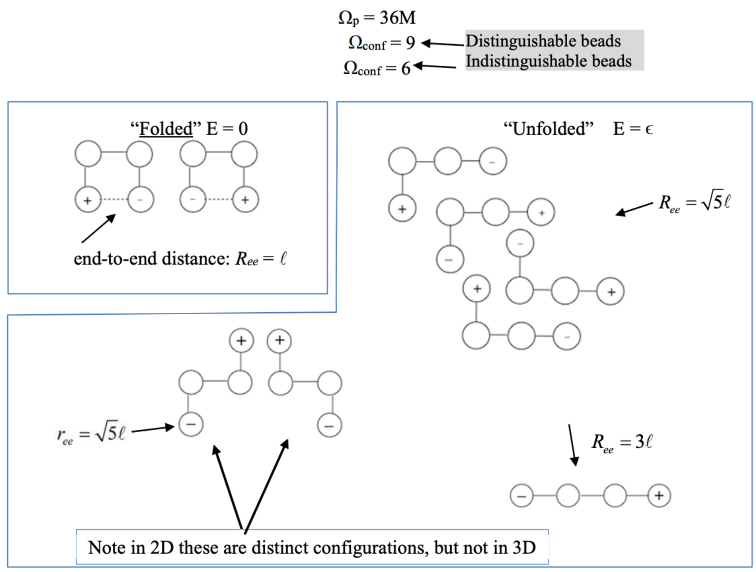
8.3: Conformational Changes with Temperature

Four bead polymer on a two-dimensional lattice

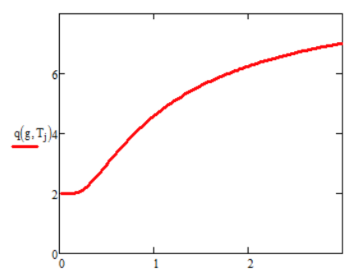


Place polymer on lattice $z = 4$ $n = 4$ in 2D (with distinguishable end beads):



Configurational Partition Function

Number of thermally accessible microstates.

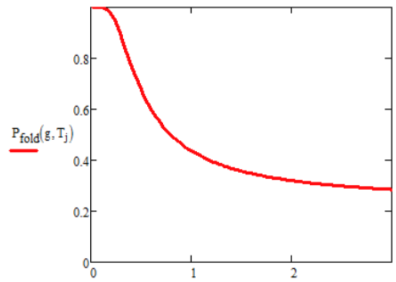


$$Q = (q_{conf})^N$$

$$\begin{aligned} q_{conf} &= \underbrace{\sum_{i\ states=1}^{9} e^{-E_i/kT}}_{\text{sum over microstates}} \\ &= \underbrace{\sum_{j\ levels=1}^{2} g_j e^{-E_j/kT}}_{\text{sum over energy levels}} \\ &= 2 + 7e^{-\varepsilon/kT} \end{aligned}$$

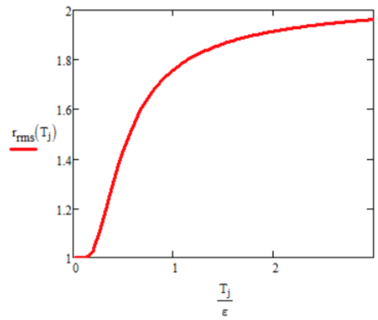
Probability of Being "Folded"

Fraction of molecules in the folded state



$$P_{fold} = \frac{g_{fold} e^{-E_{fold}/kT}}{q_{conf}} = \frac{2}{2 + 7e^{-\varepsilon/kT}}$$

Mean End-to-End Distance



$$\begin{aligned} \langle r_{ee} \rangle &= \sum_{i=1}^{9} \frac{r_i e^{-E_i/kT}}{q_{conf}} \\ &= \frac{(1)(2) + (\sqrt{5})6e^{-\varepsilon/kT} + 3e^{-\varepsilon/kT}}{q_{conf}} \\ &= \frac{2 + (6\sqrt{5} + 3)e^{-\varepsilon/kT}}{q_{conf}} \end{aligned}$$

Also, we can access other thermodynamic quantities:

$$F = -k_B T \ln Q \qquad U = \langle E \rangle = k_B T^2 \left(\frac{\partial \ln Q}{\partial T} \right)_{V,N}$$

$$S = -\left(\frac{\partial F}{\partial T} \right)_{V,N} = k_B \ln Q + k_B T \left(\frac{\partial \ln Q}{\partial T} \right)_{V,N}$$