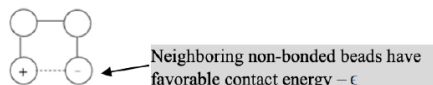
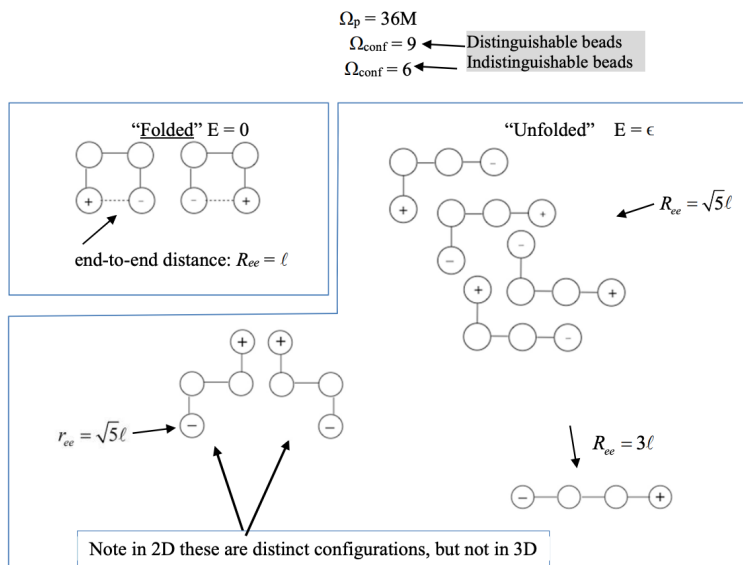


8.3: Conformational Changes with Temperature

Four bead polymer on a two-dimensional lattice

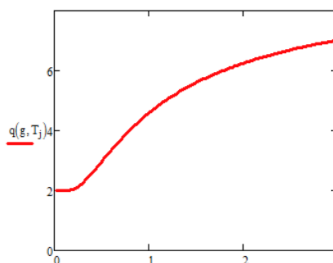


Place polymer on lattice $z = 4$ $n = 4$ in 2D (with distinguishable end beads):



Configurational Partition Function

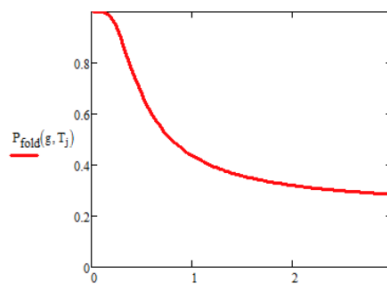
Number of thermally accessible microstates.



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

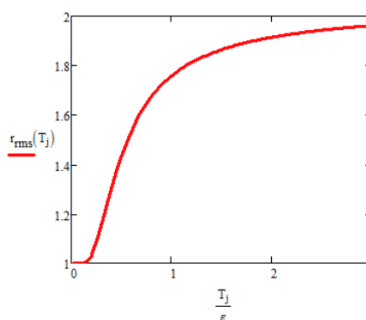
Probability of Being "Folded"

Fraction of molecules in the folded state



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

Mean End-to-End Distance



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

Also, we can access other thermodynamic quantities:

$$\begin{aligned} F &= -k_B T \ln Q \quad U = \langle E \rangle = k_B T^2 \left(\frac{\partial \ln Q}{\partial T} \right)_{V,N} \\ S &= - \left(\frac{\partial F}{\partial T} \right)_{V,N} = k_B \ln Q + k_B T \left(\frac{\partial \ln Q}{\partial T} \right)_{V,N} \end{aligned}$$

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