

8.5: Polymer–Solvent Interactions

- Use same strategy as lattice model of a fluid.
- Considering polymer (P) and solvent (S) cells:

$$U = m_{SS}\omega_{SS} + m_{PP}\omega_{PP} + m_{SP}\omega_{SP}$$

ω_{ij} = interaction energy between cells i and j
 m_{ij} = Number of contacts between i and j cells

- Number of solvent cell contacts:

$$zN_S = 2m_{SS} + m_{SP}$$

- Number of polymer cell contacts:

$$\approx (z-2) \cdot N_P \cdot n \approx z \cdot N_P n = 2m_{PP} + m_{SP}$$

\uparrow each bead connects to 2 other beads

- Mean field approximation: Substitute the average number of solvent/polymer contacts.

$$m_{SP} \approx \frac{zN_S N_P \cdot n}{M} = \langle m_{SP} \rangle$$

$$U_{\text{mix}} = k_B T \left\{ \frac{z\omega_{SS}}{2k_B T} N_S + \frac{z\omega_{PP}}{2k_B T} N_P n + \chi_{SP} \frac{N_S N_P n}{M} \right\}$$

$$\chi_{SP} = \frac{z}{k_B T} \left(\omega_{SP} - \frac{\omega_{SS} + \omega_{PP}}{2} \right) \quad \text{solvent-polymer bead exchange parameter}$$

$$\vdots$$

$$F_{\text{mix}} = N_S k_B T \ln \phi_S + N_P k_B T \ln \phi_P + \frac{z}{2} (\omega_{SS} N_S + \omega_{PP} N_P) + \chi_{SP} \frac{N_S N_P n}{M}$$

- Polymers expand in good solvents, collapse in bad solvents, retain Gaussian random coil behavior in neutral solvents (θ solvents).

Good solvents	$\chi < 0.5$	$\sqrt{\langle r^2 \rangle} \sim N^{3/5} \sim R_0 N^{3/5}$
Bad solvents (collapse)	$\chi > 0.5$	$R \sim R_0 N^{1/3}$
Theta solvents	$\chi = 0.5$	$\sqrt{\langle r^2 \rangle} \sim \frac{2N\ell^2}{3} = R_0$

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