050408 Quiz 2 Polymer Properties

a) Show that the geometric progression rule is correct. \( \sum_{k=0}^{\infty} \alpha^k = \frac{1}{1 - \alpha} \)

Then use this rule to show that a chain that does not backtrack (short range interaction) is Gaussian.

b) What is the difference between the persistence length, the Kuhn step length, the bond length and the statistical segment length (effective bond length)? How do these lengths relate to the characteristic ratio, \( C_\infty \), of Flory?

c) What is the partition function, \( Z \)? How does it relate to the probability of a system having a particular configuration of sites or elements? (Define a configuration, a system, a site or element and a state of a site.)

d) Sketch a Neumann projection for butane and show the trans, gauche+ and gauche- configurations. Plot the molecular energy versus bond rotational angle for butane based on the Neumann projection. Show that pentane contains two butane configurations.

e) For polyethylene each pair of mer units provides a pentane like structure. Sketch the Ising model for a magnetic material with 9 elements in 2D space with up and down spins and indicate the relationship between the polyethylene chain and the Ising model. Show how, in both cases, binary interaction of neighboring sites can be used to calculate the partition function.
\[ a) \quad \left( \sum_{k=0}^{\infty} x^k \right) \left( 1 - x \right) \]
\[ = \sum_{k=0}^{\infty} x^k - \sum_{k=1}^{\infty} x^k = 1 + \left( \sum_{k=1}^{\infty} x^k \sum_{k=1}^{\infty} x^k \right) \]
\[ = 1 \]

\[ \langle r_{i+1} \rangle_{stat} = \frac{r_i}{(2-1)} \quad \text{since} \quad \langle r_i \rangle_{stat} = 0 = (2-1) \langle r_i \rangle_{stat} - r_i \]

\[ \langle R^2 \rangle = \sum_{i=1}^{N} \sum_{j=1}^{N} \langle r_i \cdot r_j \rangle = \sum_{i=1}^{N} \sum_{k=0}^{\infty} \frac{b^2}{(2-1)^k} \]
\[ = N b^2 \sum_{k=0}^{\infty} \frac{2}{(2-1)^k} \]
\[ = N b^2 \left( \frac{2(2-1)}{(2-2)} \right) \]

\[ \Rightarrow \alpha = 2-1 \quad \Rightarrow \sum_{k=0}^{\infty} \frac{1}{(2-1)^k} = 1 - \frac{1}{(2-1)} \]

\[ \langle R^2 \rangle \sim N \quad \text{so it is Gaussian} \]
b) \[ C_{oo} = \frac{\langle R_0^2 \rangle}{n \ b^2} \]
\[ b = \text{bond length} / k \]
\[ 1.5 \times R \text{ for PE} \]
\[ n = \# \text{bends} \left( \frac{2 \pi \langle n_0 \rangle}{M_w} \right) \]

Statistical segment length use \( n \) and solve for \( b'_{ss} \):

\[ b'_{ss} = \left( \frac{\langle R_0^2 \rangle}{n} \right)^{1/2} = \sqrt{C_{oo} \ b^2} \]

Kuhn length assume a real step length:

\[ \text{Contour length} = n_k \ l_k \]
\[ \text{Retarded} = n_k^{1/2} \ l_k \]

\[ C_{oo} = \frac{n_k^2 \ l_k}{n \ b^2} \]

Poisson ratio \( \lambda_k \)

\[ \lambda_k = 2 \lambda_p \] (Long Chains)
\[ Z = \sum_{\text{configurations of sites}} \exp \left( \frac{\Delta E_i}{k_B T} \right) \]

System = collection of sites
Configuration = arrangement of sites of different states
Site = an element of the system that can display states

The probability of a given configuration
\[ \psi_i \]

\[ Z \]

\[ \exp \left( \frac{\Delta E_i}{k_B T} \right) \]

\[ \Delta E \]

\[ g^+ \quad g^- \]

\[ \text{Penrose} \]

\[ 0 \text{ or } 2 \text{ butons} \]
\( \psi \)

up & down spins

12 pairs of spins \( \langle \rangle \)
each pair is similar to a pentane unit of polyethylene
except that PE has 3 chains \( \overleftrightarrow{\leftrightarrow} \)

The energy for the configuration is calculated from

\[ \Delta E_i = w_0 \sum \delta_i \delta_{i+1} \]

\( \delta_i = 1 \) or \(-1\)

for majority

\( w_0 \) is energy for transition

from \( \uparrow \uparrow \) to \( \uparrow \downarrow \)

\( \Delta E_i \) can be calculated for all possible configurations