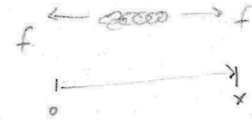
SM-2 January 2019

Polymer modeled as chain of N monomers length L_{seg}

1 Dimension

$$x = L_{seg} \sum_{i=1}^{N} \sigma_i \qquad \sigma_i = \pm 1$$



a. Construct partition function.
Calculate $\langle x \rangle$ as function of f.

Model as two level system $\quad N_\uparrow = \sum_i (\sigma_i == +1) \quad N_\downarrow = \sum_i (\sigma_i == -1) \quad N_\uparrow + N_\downarrow = N$

$$\Omega = \frac{N!}{N_\uparrow!(N-N_\uparrow)!}$$

$$x = L_{seg}(N_\uparrow - N_\downarrow) = L_{seg}(2N_\uparrow - N) \qquad W = f \cdot d = f \cdot L_{seg}$$

$$Z_1 = e^{\beta f l_{seg}} + e^{-\beta f \cdot l_{seg}} = 2\cosh(\beta f l_{seg})$$

$$Z^N = 2^N \cosh^N(\beta f L_{seg})$$

$$\langle x \rangle = \frac{-\partial G}{\partial f} \qquad G = -k_B T \ln Z = -N k_B T \ln[2\cosh(\beta f L_{seg})]$$

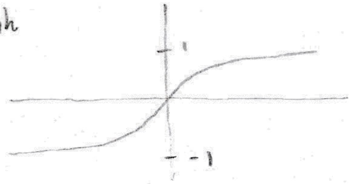
$$= N k_B T \frac{1}{2\cosh(\beta f L_{seg})} \cdot 2\sinh(\beta f L_{seg}) \cdot \beta L_{seg}$$

$$= N L_{seg} \tanh(\beta f L_{seg})$$

b. Simplify result for high force and low force.

$\langle x \rangle = N L_{seg} \tanh(\beta f L_{seg})$

tanh



$f \to \infty$ high.
$f \to 0$ low

high force $\langle x \rangle \to N L_{seg}$ makes sense, we are fully stretching the chain, low entropy limit.

low force $\langle x \rangle \to 0$ makes sense as we are not stretching chain and. it is the high entropy limit.

$$\langle x \rangle = N L_{seg} \underbrace{\frac{e^{y} - e^{-y}}{e^{y} + e^{-y}}}$$

$$\frac{1+y-1+y}{1+y+1-y} = \frac{2y}{2} = y.$$

$$\Rightarrow N L_{seg}\, y = N L_{seg} \frac{1}{K_B T} f L_{seg} = \frac{N L_{seg}^2}{K_B T} f$$ $\to$ behaves linearly for small x.

Timed ~ 40 minutes.