Homework 2
28/09/2017

An "Almost" Freely Jointed Chain

The *freely jointed chain model* consists in a sequence of n bond vectors joining $n+1$ monomers in the space. Each bond $\overrightarrow{r_i}$ has a fixed length l and there is no correlation between the directions of different vectors.

1. Evaluate the average gyration radius in the case of the *freely jointed chain model*

$$\langle R_{gyr}^2 \rangle = \left\langle \frac{1}{n+1} \sum_{i=0}^{n} (\overrightarrow{R}_i - \overrightarrow{R}_{cm})^2 \right\rangle = \left\langle \frac{1}{(n+1)^2} \sum_{i=0}^{n} \sum_{j=i}^{n} (\overrightarrow{R}_i - \overrightarrow{R}_j)^2 \ , \right\rangle \tag{1}$$

   where the centre of mass position is $\overrightarrow{R}_{cm} = \frac{1}{n+1} \sum_{j=0}^{n} \overrightarrow{R}_j$.
   Consider in particular the limit $n \gg 1$.

In the rest of this exercise we will consider a slightly modified version of this model.
Consider a chain in which the angle between two successive bonds assumes a value $\theta \in [0, \frac{\pi}{2}]$ with probability

$$p_+ = \frac{1}{2} + \epsilon \qquad \left(|\epsilon| \leq \frac{1}{2} \right) \ .$$

Remember that the direction of a vector in the space is stated by the angle $\theta \in [0, \pi]$ and a torsion angle $\phi \in [0, 2\pi]$ (see figure 1).

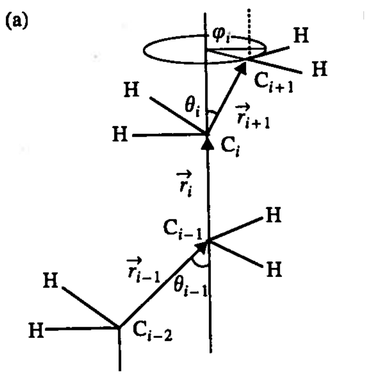

Figure 1: Freely jointed chain model (from *Polymer Physics*, M. Rubinstein and R.H. Colby).

2. Calculate the correlations $\langle \overrightarrow{r}_{i-1} \cdot \overrightarrow{r}_i \rangle$, $\langle \overrightarrow{r}_{i-1} \cdot \overrightarrow{r}_{i+1} \rangle$, and $\langle \overrightarrow{r}_i \cdot \overrightarrow{r}_j \rangle$.

3. Use the former results to evaluate the average end-to-end distance

$$R_{end}^2 = (\overrightarrow{R}_n - \overrightarrow{R}_0) \cdot (\overrightarrow{R}_n - \overrightarrow{R}_0) \ ,$$

   and the gyration radius (eq. 1). Consider in particular the limit $n \gg 1$.

Useful formulas:

$$\sum_{k=1}^{m-1} \epsilon^k = \epsilon \frac{1 - \epsilon^{m-1}}{1 - \epsilon}$$

$$\sum_{k=1}^{m-1} k\epsilon^k = \epsilon \frac{d}{d\epsilon} \sum_{k=1}^{m-1} \epsilon^k$$

$$\sum_{m=1}^{n-i} m = \frac{(n-i)(n-i+1)}{2}$$

$$\sum_{k=0}^{n} k(k+1) = \frac{n(n+1)(2n+4)}{6} \ .$$