Introduction to Biopolymer Physics

Problem 2.1

Question

Derive the expression for the radius of gyration of an ideal chain.

Solution

Consider an ideal chain with N segments and segment length l. The radius of gyration is given by

$$\langle R_g^2 \rangle = \frac{1}{N^2} \sum_{i=1}^{N-1} \sum_{j=2}^{N} \langle h_{ij}^2 \rangle \qquad \text{with} \quad j > i, \tag{1}$$

where $\langle h_{ij}^2 \rangle$ is the mean square distance between segments i and j

$$\langle h_{ij}^2 \rangle = (j - i)\, l^2. \tag{2}$$

Hence, the radius of gyration can be written as

$$\langle R_g^2 \rangle = \frac{l^2}{N^2} \sum_{i=1}^{N-1} \sum_{j=2}^{N} (j - i) = \frac{l^2}{N^2} \sum_{i=1}^{N-1} \sum_{x=1}^{N-i} x. \tag{3}$$

To solve this double summation, we consider the following results:

$$\sum_{k=1}^{n} 1 = n \tag{4}$$

$$\sum_{k=1}^{n} k = \frac{n(n+1)}{2} \tag{5}$$

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

With eqn. (5) one summation of eqn. (3) can be evaluated, and we get

$$\langle R_g^2 \rangle = \frac{l^2}{N^2} \sum_{i=1}^{N-1} \frac{(N-i)(N-i+1)}{2} \tag{7}$$

$$= \frac{l^2}{2N^2} \sum_{i=1}^{N-1} \left(\underbrace{N^2 + N}_{a} - \underbrace{i\,(2N+1)}_{b} + \underbrace{i^2}_{c} \right) \tag{8}$$

The sums over the three terms a,b and c can be evaluated individually, using eqn.(4)-(6), yielding the following results:

$$\frac{l^2}{2N^2}\sum_{i=1}^{N-1} N^2+N = l^2\,\frac{(N^2+N)(N-1)}{2N^2} \tag{9}$$

$$-\frac{l^2}{2N^2}\sum_{i=1}^{N-1} i\,(2N+1) = -l^2\,\frac{(2N+1)(N-1)N}{4N^2} \tag{10}$$

$$\frac{l^2}{2N^2}\sum_{i=1}^{N-1} i^2 = l^2\,\frac{(N-1)N(2N-1)}{12N^2} \tag{11}$$

Collecting the terms proportional to N yields

$$\langle R_g^2\rangle = l^2\left(\frac{N}{2}-\frac{N}{2}+\frac{N}{6}\right)=\frac{N\,l^2}{6}. \tag{12}$$

As all other terms are of order 1 or N^{-1}, they can be neglected for large polymer chains.