Tutorial (March, 8 2018)

1) Average gyration radius of the ideal Gaussian chain – The average square gyration radius, $\langle R_g^2 \rangle$, of a polymer chain made of N monomers is defined by the formula:

$$\langle R_g^2 \rangle \equiv \left\langle \frac{1}{N} \sum_{i=1}^{N} (\vec{r}_i - \vec{r}_{cm})^2 \right\rangle , \tag{1}$$

where $\vec{r}_{cm} \equiv \frac{1}{N} \sum_{i=1}^{N} \vec{r}_i$ is the chain center of mass and $\langle \cdot \rangle$ means average over all possible polymer conformations.

1. Demonstrate that $\langle R_g^2 \rangle = \left\langle \frac{1}{2N^2} \sum_{i=1}^{N} \sum_{j=1}^{N} (\vec{r}_i - \vec{r}_j)^2 \right\rangle$.

2. By using the known relation for the Gaussian chain $\langle (\vec{r}_i - \vec{r}_j)^2 \rangle = b^2 |i - j|$, calculate the corresponding exact expression for $\langle R_g^2 \rangle$ and demonstrate that $\lim_{N \to \infty} \langle R_g^2 \rangle = \frac{b^2 N}{6}$

2) Structure factor of the ideal Gaussian chain – The average static structure factor $\langle S(\mathbf{q}) \rangle$ describes how a certain material scatters incident radiation with wave number $\mathbf{q}$. For a polymer chain made of N monomers, $\langle S(\mathbf{q}) \rangle$ is defined by the formula:

$$\langle S(\mathbf{q}) \rangle \equiv \left\langle \frac{1}{N^2} \sum_{i=1}^{N} \sum_{i=1}^{N} e^{i\mathbf{q} \cdot (\mathbf{r}_i - \mathbf{r}_j)} \right\rangle , \tag{2}$$

where $\langle \cdot \rangle$ means average over all possible polymer conformations.

1. Calculate the exact $\langle S(\mathbf{q}) \rangle$ for the Gaussian chain, and derive the corresponding small-$\mathbf{q}$ and large-$\mathbf{q}$ limits.

2. By using the previous results, propose a heuristic expression for $\langle S(\mathbf{q}) \rangle$ which gives the same small-$\mathbf{q}$ and large-$\mathbf{q}$ limits. Find its corresponding expression in real space.