Solution 4

Worm-like Chain Model

The first remark is that the *freely rotating chain model* is similar to the model of homework 2, but the angle between consecutive bonds is now fixed to the value θ. Repeating the calculation, it is easy to prove that

$$\langle \vec{r}_{i-1} \cdot \vec{r}_i \rangle = l^2 \cos\theta$$
$$\langle \vec{r}_i \cdot \vec{r}_j \rangle = l^2 (\cos\theta)^{|i-j|} = l^2 e^{-\frac{|i-j|}{s_p}} \ ,$$

where l is the length bond, and $s_p = -\frac{1}{\log(\cos\theta)}$ is the *persistent scale*. Accordingly, the *persistence length* is

$$l_p = l s_p = -\frac{l}{\log(\cos\theta)} \overset{\theta \ll 1}{\approx} -\frac{l}{\log(1-\frac{\theta^2}{2})} \overset{\theta \ll 1}{\approx} \frac{2l}{\theta^2} \ .$$

In the *worm-like chain model* $l \to 0$, $\theta \to 0$ while the ratio $\frac{l}{\theta^2}$ is kept fixed. When $l \to 0$ the chain becomes *continuous* and the index i counting the bonds is replaced by the distance $u = il$. In the calculation of the mean square end-to-end distance the sums are replaced by integrals:

$$\begin{aligned}
\langle R_{end}^2 \rangle &= \sum_{i=1}^{n}\sum_{j=1}^{n} \langle \vec{r}_i \cdot \vec{r}_j \rangle = l^2 \sum_{i=1}^{n}\sum_{j=1}^{n} e^{-\frac{|i-j|l}{l_p}} \longrightarrow \int_0^{R_{max}} du \int_0^{R_{max}} dv\, e^{-\frac{|u-v|}{l_p}} \\
&= \int_0^{R_{max}} du \left[\int_0^u e^{-\frac{u-v}{l_p}} dv + \int_u^{R_{max}} e^{-\frac{v-u}{l_p}} dv \right] \\
&= \int_0^{R_{max}} du \left[e^{-\frac{u}{l_p}} l_p \left\{ e^{\frac{u}{l_p}} - 1 \right\} + e^{\frac{u}{l_p}} (-l_p) \left\{ e^{-\frac{R_{max}}{l_p}} - e^{-\frac{u}{l_p}} \right\} \right] \\
&= 2 l_p R_{max} - 2 l_p^2 \left[1 - e^{-\frac{R_{max}}{l_p}} \right] \ .
\end{aligned}$$

1. If $R_{max} \gg l_p$ then $\langle R_{end}^2 \rangle \approx 2 l_p R_{max} - 2 l_p^2 \approx 2 l_p R_{max}$
2. If $R_{max} \ll l_p$ then $\langle R_{end}^2 \rangle \approx 2 l_p R_{max} - 2 l_p^2 \left[1 - 1 + \frac{R_{max}}{l_p} - \frac{1}{2}\frac{R_{max}^2}{l_p^2} \right] \approx R_{max}^2$

A fractal dimension

We are interested in computing the fractal dimension

$$D = -\frac{\log(L(a')/L(a))}{\log(a'/a)} \ ,$$

where $L(a')$ is the size (e.g. length, area, and etc.) of the fractal measured with the scale length a', and similarly $L(a)$ is the size of the fractal measured with the scale length a.

1. If we measure a straight line with two rules of length a, and $a' = 10\,a$ we get $L(a) = 10\,L(a')$ (think of measuring a table in *cm* or in *mm*), therefore $D = 1$, as we expected;

2. The Koch snow-flake: with a ruler 3 times smaller we will measure a length 4 times bigger, so $D = \frac{\log 4}{\log 3} \sim 1.26$, which is more than how a 1 dimensional object would behave;

3. The Sierpinski gasket: with a triangle of edge 2 times smaller we will measure a surface 3 times bigger, then $D = \frac{\log 3}{\log 2} \sim 1.58$, which is less than the expected behavior of a 2 dimensional object;

4. The Menger sponge: reducing the square edge of a factor 3 we will measure a volume 20 times bigger, therefore $D = \frac{\log 20}{\log 3} \sim 2.73$;

5. Let a be a length scale satisfying $b \ll a \ll R_{e-e}$. If we try to cover the random walk with a ruler of length a, at each step we will be measuring the end-to-end distance of a part of the original chain. Since $a \gg b$, such a part still satisfies random walk statistics, so that $a \sim n^{1/2}$, where n is the (expected) number of bonds composing the part of the random walk we are looking at. By inverting this relation, we find

$$n \sim a^2 \tag{1}$$

Since the total number of bonds in the chain is N, we need to repeat the operation N/n times in order to cover the entire walk. In other words, $N/n = Na^{-2}$ is the measure of the chain length when using a ruler of length a. By repeating the same procedure with a different length scale a', we end up with a measure Na'^{-2}. By applying the definition, we thus find

$$D = -\frac{\log \frac{Na'^{-2}}{Na^{-2}}}{\log \frac{a'}{a}} = -\frac{\log \left(\frac{a'}{a}\right)^{-2}}{\log \frac{a'}{a}} = 2 \tag{2}$$