

Homework 4

Worm-like Chain Model

The *persistence length* l_p of a polymer chain is defined by the relation

$$\langle \vec{r}_i \cdot \vec{r}_j \rangle \equiv l^2 e^{-l|i-j|/l_p}, \quad (1)$$

When the distance $l|i-j|$ between the bond vectors i and j becomes much greater than l_p , \vec{r}_i and \vec{r}_j are essentially uncorrelated, so that l_p can be seen as a measure of the stiffness of the polymer.

- Calculate l_p for a Freely Rotating Chain (FRC) with fixed bond angle θ and bond length l . Show that for small values of the bond angle $l_p \approx \frac{2l}{\theta^2}$.

The *Worm-Like Chain* (WLC) is a continuum model of a polymer chain, where the polymer is seen as a continuous line. Such a model can be obtained as a limit case of several possible discrete models. In the case at study, the WLC is obtained by considering a FRC and taking the limit for $l \rightarrow 0$ and $\theta \rightarrow 0$ at constant persistence length. Consistently, the number of bonds n suitably grows, in order to keep constant the maximum end-to-end distance $R_{max} = nl \cos(\theta/2) \approx nl$, which represents now the contour length of the chain.

- Show that the mean square end-to-end distance $\langle R_{end}^2 \rangle = \sum_{i=1}^n \sum_{j=1}^n \langle \vec{r}_i \cdot \vec{r}_j \rangle$ as a function of R_{max} and l_p is

$$\langle R_{end}^2 \rangle = 2l_p R_{max} - 2l_p^2 \left[1 - e^{-\frac{R_{max}}{l_p}} \right] \quad (2)$$

Hints: use the expression containing l_p for the correlation $\langle \vec{r}_i \cdot \vec{r}_j \rangle$ and recall that the continuous limit of the summation is an integration, e.g.

$$l \sum_{i=1}^n \rightarrow \int_0^{R_{max}} du.$$

- Find a simplified expression of eqn (2) in the two limits $R_{max} \gg l_p$ and $R_{max} \ll l_p$. What is their physical interpretation?

A fractal dimension

A fractal is broadly speaking a *self similar* object, i.e. it looks alike on all length scales. Therefore, it is not possible to define a characteristic scale, nor it is possible to determine at which scale a fractal is being viewed. A crucial property of each fractal is its *dimension*, which describes how it *fills* its embedding space. An intuitive¹ definition of fractal dimension is the following

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

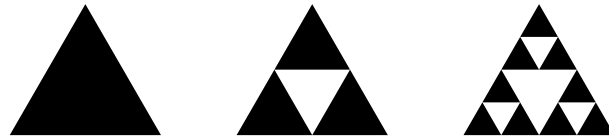
where $L(a')$ is the size (e.g. length, area, and etc.) of the fractal measured with the length scale a' , and similarly $L(a)$ is the size of the fractal measured with the length scale a . Note that this equation implies $L(a) \sim a^{-D}$.

¹For an extensive discussion about fractal dimension see for example *Fractal Geometry*, K. Falconer, John Wiley & Sons, 2nd edition (2003).

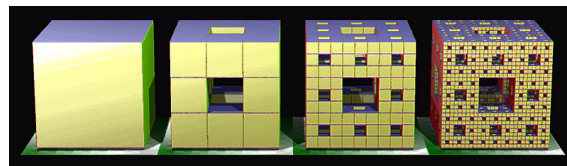
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1. What is D for a straight line?
 2. What is D for a von Koch snow-flake? It is built from a line segment of unit length by replacing at each step the middle third of each straight line by the other two sides of an equilateral triangle (see below).



3. What is D for the Sierpinski gasket? It is obtained by repeatedly removing inverted equilateral triangles from an initial equilateral triangle of unit side length (see below).



4. What is D for the Menger sponge? It is built from a cube of unit side length by iteratively dividing the faces into 9 squares, and by removing the cube at the middle of every face together with the cube in the center (see below).



5. In the case of a polymer, strictly speaking it is not true that scale invariance holds at all possible scales. Indeed, there is a lower bound given by the bond length b and an upper bound given by the end to end distance R_{e-e} . However, provided we are looking at length scales larger than b and smaller than R_{e-e} , chain models show scale invariance, so that under such an assumption it makes sense to treat them as fractal objects².

What is D for a random walk? (Use $R_{e-e} \sim N^{1/2}$ and consider a part of the entire random walk formed by n steps).

²Nevertheless, they are not fractal in the same sense as the previous examples, where a perfect scale invariance is seen. In the case of a random walk, given a realization it will look different at different scales. What are invariant in this case are the statistical properties of the polymer, so that sometimes one refers to polymers as *statistical fractals*, to distinguish them from the fractals following more strictly the definition.