BCHM485 Quiz #5 Spring 07

1. There are many ways to characterize the end-to-end distance for a polymer chain. Some of them we covered in class, but some you might want to calculate yourself. For a freely-jointed 3D polymer chain of N segments of length b calculate and compare the following characteristics (all of them have the dimension of a length, hence could be used as a measure of the distance!):

(A) The root-mean-square end-to-end distance, $\langle L^2\rangle^{1/2}$
(B) The average end-to-end distance, $\langle L\rangle$
(C) The most probable end-to-end distance
(D) Another measure, $\langle L^3\rangle^{1/3}$

2. Answer the same questions as in Problem 1 but for a 1D chain model (1D random walk model).

3. Assume a polymer chains fully absorbed on a plane surface – this will make the chain a 2D chain. Will the end-to-end distance become greater or smaller than for the 3D or 1D chain? Answer the questions in Problem 1 and compare the results with those in Problems 1 and 2.

4. A hypothetical polymer chain of 100 segments of length b = 3 Å has the root-mean-square end-to-end distance of 100 Å. Answer the following questions:

(A) Does it behave as an ideal freely-jointed chain? Explain your reasoning and support it by calculations.
(B) Calculate the number of Kuhn's statistical segments in the chain and the Kuhn's statistical segment length. (this material will be covered on Tue)

5. The genome of T2 bacteriophage is $1.7\ 10^5$ nucleotides long. Assume you have a linear piece of DNA of this length, and this DNA adopts a random coil conformation. The Kuhn's statistical segment length for DNA is 120 nm, and the base-pair spacing along the DNA is 0.34 nm. Use these data to answer the following questions

(A) Determine the root-mean-square end-to-end distance for a random coil that a DNA of this length can form, assuming it behaves as an ideal freely-jointed chain with b = 0.34 nm. What is the size (radius of gyration R_G) of this random coil?
(B) Determine the root-mean-square end-to-end distance and R_G for a random coil that this DNA can form under "real" conditions, i.e. when it behaves as an ideal freely-jointed

chain with *b* being the Kuhn's statistical segment length. Compare your answer with that in (A).

Practical advices how to calculate the relevant integrals.

In Problems 1-3 and most problems of this kind you deal with integrals of the following form (or can be rearranged to have this form): $I = \int_0^\infty e^{-\frac{L^2}{A^2}} L^a dL$, where A is a constant with respect to *L* (for example, $A^2=2Nb^2/3$ for a 3D chain) and *a* is an integer . It is often useful to follow these steps:

Step 1. Get rid of A under the integral. Introduce a new variable, for example, x = L/A. This gives $I = A^{a+1}\int_0^\infty e^{-x^2} x^a dx$, thus the dependence of the result on N or any other parameters that are included in *A* becomes obvious, and the integral itself is just a number (!). If you are interested in the dependence of *I* on A (or N or *b* etc) – this is already your answer.

Step 2. If you need the exact numeric answer, then you have to actually calculate $\int_0^\infty e^{-x^2} x^a dx$.

There are two possibilities, depending on *a*.

1. ***a*** is an **odd** number, $a = 2n+1$. Then it is useful to introduce a new variable, e.g. $y = x^2$, such that $dy = 2x\,dx$. This will allow you to get rid of the square (x^2) in the exponential, and the integral becomes $\frac{1}{2}\int_0^\infty e^{-y} y^n dy$, where $n = (a-1)/2$, and now everything is simple, because you can apply calculation by parts or use the known formula, $\int_0^\infty e^{-y} y^n dy = n!$, to calculate this integral.

2. ***a*** is an **even** number, $a = 2n$. In this case the trick we used above won't help, but you can use the formula $\int_0^\infty e^{-y^2} y^{2n} dy = (-1)^n \frac{\sqrt{\pi}}{2}\left[\frac{d^n}{dz^n}\left(z^{-\frac{1}{2}}\right)\right]_{z=1} = \frac{\sqrt{\pi}}{2}\frac{1\cdot 3\cdot 5\cdot\ldots\cdot(2n-1)}{2^n}$, which gives

$\int_0^\infty e^{-y^2} y^2 dy = \frac{\sqrt{\pi}}{4}$; $\int_0^\infty e^{-y^2} y^4 dy = \frac{3\sqrt{\pi}}{8}$; etc.

For those of you interested in how I pulled this rabbit out of a hat, the formula shown above is obtained by realizing that $y^{2n}e^{-y^2}$ can be represented as a result of *n*-times differentiation of e^{-zy^2} over *z*, if *z* is set to *z*=1 in the end:

$y^{2n}e^{-y^2} = (-1)^n \left[\frac{d^n}{dz^n} e^{-zy^2} \right]_{z=1}$. Then you get $\int\limits_0^\infty y^{2n}e^{-y^2}\,dy = (-1)^n \left[\frac{d^n}{dz^n} \int\limits_0^\infty e^{-zy^2}\,dy \right]_{z=1}$, which gives you the formula above because $\int\limits_0^\infty e^{-zy^2}\,dy = \frac{\sqrt{\pi}}{2\sqrt{z}}$.