Name: PHY401 (Spring 2010), 03/31/10

Homework Assignment #7

(*Due Date*: Friday, April 09, 10:20 am, in class)

7.1 *2D Random Walk* (cf. Exercise 7.2 in the textbook) *(2+2 pts.)*
Write a FORTRAN program to simulate a random walker in 2 dimensions, taking steps of unit length in $\pm x$ or $\pm y$ direction on a discrete square lattice.

(a) Plot $\langle x_n \rangle$ and $\langle (x_n)^2 \rangle$ up to n=100 by averaging over at least n_w=10^4 different walks for each $n > 3$.

(b) Show that the motion is diffusive, $\langle r^2 \rangle \propto t$, and determine the value of the diffusion constant (an “eyeball” fit to your numerical data is ok).

7.2 *2D Self-Avoiding Walk* (cf. Ex. 7.5 in the textbook) *(2+2+2 pts.)*
Write a FORTRAN program to simulate 2D self-avoiding walks (SAWs) using the “trial” method discussed in class. Make sure that each walk of given step-length n (polymer with given molecule number, n) has the same probability i.e., each step direction should always be selected with probability 1/3 (except for the first step).

(a) Defining C_n as the total number of distinct SAWs for n steps, the probability for a single SAW simulation surviving after n steps is given by

$$P(n) = \frac{C_n}{3^n} \tag{1}$$

which quantifies the numerical attrition in simulating SAWs. Compute (and plot) $P(n)$ up to n=50 by conducting $\sim 10^6$ trials for each n. Comment on a comparison to the exact results quoted in Table 7.1 of the textbook.

(b) Suppose the large-n behavior of C_n is parameterized by

$$C_n \simeq C_0 \; \mu^n \; n^{\gamma-1} \tag{2}$$

with parameters $\mu < 3$ (why?) and γ. Show analytically that

$$\frac{P(n+1)}{P(n)} \simeq \frac{\mu}{3}(1 + \frac{\gamma-1}{n}) \tag{3}$$

and plot this relation for your data as a function of $1/n$ to estimate μ and γ.

(c) To investigate the diffusive properties of the 2D SAW show analytically that

$$\frac{\langle r^2_{n+1} \rangle}{\langle r^2_n \rangle} = 1 + 2\nu\frac{1}{n} \tag{4}$$

for large n using the definition of the Flory exponent, ν,

$$\sqrt{\langle r^2(t) \rangle} \equiv A\, t^\nu \;, \;\; t \text{ large.} \tag{5}$$

Use the relation (4) to plot your 2D SAW data and determine the value of the Flory exponent.