Name: PHY401 (Spring 2013), 03/26/13

Homework Assignment #7

(*Due Date*: Tuesday, April 02, 05:30 pm, in class)

7.1 *Flory Exponent in Random/Self-Avoiding Walks* (cf. Ex. 7.5 in textbook) *(2+2+2 pts.)*
Write a FORTRAN code to simulate random walks on a 2D square lattice starting from the origin.

(a) Simulate unrestricted random walks up to n=100 steps, averaging over $n_w \simeq 2 \cdot 10^4$ walks for each $n > 3$. Plot $\langle r_n^2 \rangle$ as function of n ($r^2 = x^2 + y^2$), and extract the Flory exponent in $\sqrt{\langle r^2 \rangle} \equiv A\ t^\nu$ (t large), by an eyeball fit.

(b) Simulate a 2D self-avoiding random walk 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). Plot $\langle r_n^2 \rangle$ vs. n. Go to at least n=50 and use a sufficiently large n_w. To extract the Flory exponent, first show analytically that

$$\frac{\langle r_{n+1}^2 \rangle}{\langle r_n^2 \rangle} = 1 + 2\nu \frac{1}{n} \qquad (1)$$

for large n. Replot your 2D SAW data using this relation and determine the value of ν by an eyeball fit. Re-evaluate ν from part (a) with this technique.

(b) Investigate fluctuations of the 2D random walk by extracting the variance, $\Delta(r_n^2)$, as function of n. Evaluate the exponent x in $\sigma(t) \equiv \sqrt{\Delta(r^2(t))} \propto t^x$ by the same technique as in part (b). Sketch the result as a "1-σ" band around $\langle r^2 \rangle$ from part (a).

7.2 *Diffusion and Central Limit Theorem* (cf. Ex. 7.9 in textbook) *(3+1 pts.)*
Write a FORTRAN program to solve the 1-D diffusion equation using the finite difference method with diffusion constant D=2. Start from an initial density profile (e.g., box profile) that is sharply peaked around x=0 but still extends over a finite number of grid sites, e.g., 1000 particles in each of the four bins from $x = -2$ to $+2$.

(a) Plot time snapshots of the density distribution when significant changes of the latter have occurred, and show that at later times it can be described a one-parameter fit of a normal distribution.

(b) Plot the extracted width, σ, of the distribution as a function of time and compare it to the expected theoretical behavior (plot the latter as a separate line).