

Name:

PHY401 (Fall 2006), 10/25/06

Last 4 digits of UIN:

Score:

## Homework Assignment #7

(Due Date: Wednesday, November 08, 12:40 pm, in class)

7.1 *3-D Self-Avoiding Walk* (cf. Exercise 7.6 in the textbook) (4 pts.)

Write a FORTRAN program to simulate a self-avoiding random walk in 3 dimensions, taking steps of unit length in  $x$ -,  $y$ - or  $z$ -direction. In particular, make sure that each walk of step-length  $n$  (polymer with given molecule no.  $n$ ) has the same probability. Show that the motion (polymer size) is diffusive with  $\sqrt{\langle r^2 \rangle} = At^\nu$ ; determine the value of the Flory exponent  $\nu$  (you can use either the statistical “trial” method or the exact depth-first enumeration method for your computation).

7.2 *Diffusion Limited Aggregation and Fractal Dimension* (cf. Ex. 7.19) (5 pts.)

- (a) Write a FORTRAN program to generate DLA clusters in 3 dimensions. To save computer time, implement the following features into your simulation: start from a seed at the origin, let random walkers start from a random position on a circle (but on your numerical grid) about 8-10 units away from the origin. When growing the cluster, keep the circle about 5 units away from the perimeter of the cluster. If a walker has wandered off to more than 1.5 times the starting radius, terminate the walk and begin a new one. Grow several clusters to a size of several ten-thousands attachments.
- (b) Calculate the dimensionality of the clusters you have generated in part (a) by finding the exponent,  $d_f$ , in the mass radius relationship,  $m(r) \propto r^{d_f}$ , and evaluate the average  $d_f$  as your best estimate for the dimensionality of the DLA cluster.

7.3 *2-D Percolation and Critical Exponent* (cf. Figs. 7.26, 7.27, Ex. 7.31) (6 pts.)

- (a) Write a FORTRAN program to simulate the percolation transition on a  $N \times N$  lattice by subsequently (randomly) filling lattice sites corresponding to an increase in occupation probability,  $p$ . Determine the critical probability  $p_c$  by checking, after each new entry, for the first appearance of a spanning cluster, and plot the spanning cluster (cf. Fig. 7.28 in the textbook). Repeat this procedure for various lattice sizes  $N$  (e.g.  $N=10$  to 40 in steps of 5) and plot  $p_c(N^{-1})$  to extrapolate to the infinite-size limit,  $p_c(0)$ .
- (b) Starting from a single “seed” site, use the breadth-first growth algorithm to generate a percolating (2-D) cluster for various site occupation probabilities  $p < p_c = 0.593$  (the growth should always terminate itself). For each  $p$ , estimate the “correlation length”,  $\xi(p)$ , by computing the average distance of all cluster sites from the initial seed site. Fit  $\xi(p)$  with a power law  $\xi \propto |p - p_c|^{-\nu}$  in order to estimate the critical exponent  $\nu$ .