Homework 2
Due 4/27/10

This homework has a range of problems, both numerical and analytical. Do what problems you find interesting and that you feel are doable. If you can't understand a problem, please feel free to ask.

Problem 1 is quite short and should be possible for everyone to at least attempt.

Problem 2 is also not too difficult but a little bit longer. The result should be similar to the discussion of de Gennes.

Problem 3 is numerical and should not be too long. Make sure that you do binning in the same program. Do not print out results to another program to do the histogram.

Problems 4 requires a fairly high degree of familiarity with statistical mechanics. It is not that long, but requires understanding partition functions quite well.

Problem 5 is a nice application of scaling theory but requires quite a good understanding of it. It is not long, but you have to be familiar with the kind of arguments used in de Gennes to do it.

Problem 6 is numerical and can be the starting point for lots of neat simulations of polymers. It should require several 100 lines of C code to implement.

1. Consider an ideal ring polymer, that is one with no interactions, topological or otherwise. It is composed of N beads with positions $(\mathbf{r}_1, \ldots, \mathbf{r}_N)$. Consider $\langle |\mathbf{r}_{N/2} - \mathbf{r}_1|^2 \rangle$. Consider the same quantity when the bond between beads 1 and N are cut giving a linear chain. Calculate the ratio of these two quantities.

2. Consider an infinitely long ideal polymer chain in three dimensions with a step length l. If a monomer is at position $\mathbf{r}_0$, calculate the probability density that another monomer with be at position $\mathbf{r}$. Assume that $r >> l$, that is don't worry about short distance effects of order the chain step length. You can get the form of the result in any dimension but don't have to. *Hint: The answer is the sum of probabilities for different arclengths. This sum can be approximated by an integral. The integral can be done by Fourier transformation with respect to* $\mathbf{r}$. *It can also done by a change of variables if you're working in three dimensions.*

3. Verify your results for problem 2 numerically. The statistics can be improved by binning over spherical shells, but it is not necessary for you to do this.

a Write a function to generate a random walk of N steps.

b Keep track of the number of times it hits a site on the lattice by including a *density map* in the form of a three dimensional array, or a one dimensional array if you're binning over spherical shells.

c By calling the random walk function repeatedly, the density map becomes smoother.

d By looking along the x direction, after sufficiently many runs, you can compare your answer to the analytical result. Alternatively if you're binning over spherical shells you can get the answer by examining the one dimensional array.

Alternatively, you can use SciPy to do this in a small number of lines of code, though not quite as efficiently as in a language like C. Here is a hints file: `http://physics.ucsc.edu/~josh/120.10/home2/ideal_density_hints.py`.

4. *SAW in a bath of monomers.* Consider a self avoiding walk in bath of monomers on a lattice in d dimensions. A "Monomer" occupies a single lattice site. We specify the interaction of the polymer with the bath of monomers as follows: a point on the polymer has an energy e of interaction with a monomer when they both occupy the same lattice site, otherwise they do not interact. The monomers can be taken to be at constant chemical potential μ (the "Grand Canonical Ensemble"). That is, if we denote a lattice site by $\mathbf{R}$, the site is occupied if $n(\mathbf{R}) = 1$, otherwise it is 0. The energy (Hamiltonian) of the system has to have an additional term $-\mu N$ added to it, where N is the number of monomers in the system. How do these monomers effect the chain's statistics? To figure this out, keep the conformation of a polymer chain fixed, but calculate the partition function for the solvent monomers. How does your answer depend on the conformation of the polymer chain?

5. *SAW in a bath of rods.* Consider a three dimensional SAW in a bath of rods that all are aligned in the z direction and are taken to be infinitely long. Use scaling theory to calculate what the statistics of the chain look like. Assume that the chains will be elongated in the z direction, and calculate how the radius of gyration in the $x - y$ plane and in the vertical direction scale with N. Take the density of rods per unit area to be ρ.

a What is the (two dimensional) pressure exerted by a gas of rods?

b How does the change in free energy scale when an area A is made vacant of rods?

c The polymer will occupy a tube along the z direction. If the polymer dimensions in th $x - y$ direction R_{xy} is given, what is the reduction in entropy of the SAW.

d Adding together both effects [b] and [c], calculate R_{xy}

e How does R_z scale with R_{xy}?

6. *Reptation dynamics for an SAW.* Implement code to simulate a SAW using "reptation dynamics". This describes an iteration of the algorithm:

a Pick the end of a chain at random.

b Try the following move: Cut off a monomer and add it to the other side going in a random direction. If it lands in on an occupied site, reject the move, otherwise accept it.

Points to keep in mind: You will want to use a "density map" to do the checking of occupation. It is better not to shift over the whole array of coordinates at every step. Keep track of the index of the head and tail in coordinate array and move that instead of shifting the whole array. Estimate how the equilibration time scales with chain length. Can you obtain ν? You can do this in two or three dimensions. It is easiest to implement this algorithm using "skew boundary conditions" that will be discussed in class.