Homework 3
Due 5/6/10

This assignment has three aims. The first is to get more familiar with stochastic equations and how to look at them directly or in terms of their probability distribution. The second is to better understand how random walks and polymer chains differ when interacting with boundaries. You'll try to understand this in problems 5 and 6. Problems 7 and 8 explore the solution to stochastic equations numerically.

1. Consider the Langevin equation for a particle with strong damping under the influence of a random force:

$$\frac{dx}{dt} = f(t)$$

Where $f(t)$ is a random function with mean zero and $\langle f(t)f(t')\rangle = \delta(t-t')$. Calculate $\langle (x(t)-x(0))^2\rangle$. The average is over all possible realizations of the random function f. *Hint: Solve for $x(t)-x(0)$ to get an answer in terms of $f(t)$. Then square and average the result. Interchange order of integration of average.*

2. The Langevin equation in problem 1 has a probability distribution for position x and time t that satisfies the diffusion equation

$$2\frac{\partial P(x,t)}{\partial t} = \frac{\partial^2 P(x,t)}{\partial x^2}$$

Assume the particle starts out at the origin, that is $P(x,0) = \delta(x)$, solve for $P(x,t)$ and compare your answer to problem 1. Generalize this to where the particle starts out at position $x = l$.

Hint: Fourier transform with respect to x giving a function $\hat{P}(k,t)$. This will give a first order ordinary differential equation. The solution has one arbitrary constant that depends on k, $a(k)$. Obtain $a(k)$ using the initial condition and back transform.

3. The current of particles going past a point x $j(x)$ satisfies

$$\frac{\partial j}{\partial x} = -\frac{\partial P}{\partial t}$$

This is just a consequence of conservation of mass.

(a) Show that $j = -\frac{1}{2}(\partial P/\partial x)$, gives the diffusion equation of problem 2.

(b) Suppose there is an impenetrable boundary at $x = 0$. What is boundary condition at this point? This is called a "reflecting" boundary condition.

(c) A particle starts out at $x = l$ satisfying the Langevin equation of problem 1. There is an impenetrable wall at $x = 0$. Using the boundary condition from part (b) and the solution to the last problem, calculate the probability distribution for position x and time t. *Hint: use the "method of images" to solve the diffusion equation so that you have appropriate boundary condition at $x = 0$.*

4. Instead of 3(b), we have a totally absorbing boundary at $x = 0$. In this case, all particles hitting this boundary vanish. The appropriate boundary condition here is $P(x = 0, t) = 0$. Calculate the probability distribution for position x and time t, in this case.

5. Consider a polymer chain in one dimension of length L. Its path is a random walk as in problem 1, but with time replaced with arclength, that is $t \to s$. Assume that the polymer is held fixed at $x = l$ and assume that there is an impenetrable barrier at $x = 0$.

(a) Calculate the probability distribution of the end to end distance. You may leave the normalization as an integral.

(b) The answer simplifies when L becomes very large. Calculate the limiting form in this case.

Hint. The probability distribution is given by statistical mechanics. If the chain goes back and forth with fixed step length, then all configurations are equally likely except those that cross the origin. Paths that cross the origin have a statistical weight of zero.

6. Now use this to understand how to correctly describe the growth of a self avoiding walk. A "true self-avoiding walk" is one that grows a single step at a time but rejects moves that collide with itself. Is this more akin to an absorbing or reflecting boundary condition? What boundary condition would correspond to a self-avoiding walk?

7. Consider a particle in an optical trap. A good approximation for its motion is similar to that of problem 1, a Langevin equation of the form

$$\frac{dx}{dt} = f(t) + f_{trap}(x)$$

but there is now an additional linear restoring force $f_{trap}(x) = -kx$ where k is the effective spring of the trap. You can solve this problem numerically to obtain the equilibrium distribution function for x, and the correlation function $\langle x(0)x(t) \rangle$. This is done in the file: `http://physics.ucsc.edu/~josh/120.10/home3/harmonic.py`. Run it to obtain the above quantities. Explain the results that you obtain.

8. Many problems involve motion in a potential with more than one equilibrium point. Consider motion in a "double well" potential. A recent example is the study of molecular unfolding by applying an external force to a single molecule. This kind of problem is analyzed in this hints file: `http://physics.ucsc.edu/~josh/120.10/home3/nonlinear_hints.py`. It solves the Langevin equation of problem 7 numerically for the case where $f_{trap}(x)$ has two stable equilibrium points.

(a) The potential is given in that file. Complete the code to obtain the force $f_{trap}(x)$.

(b) We also know that in thermal equilibrium, the probability of finding the particle at position x is given by the Gibbs distribution. The rest of the code compares the simulation results with the exact result from the Gibbs distribution. Fill in the rest of the code using the suggestions provided in the comments.

(c) Run the code and compare the analytic and numerical solution.

(d) Now lower the temperature to 0.01. What happens now? Do the analytical and numerical results agree? If not, why not?