

Homework 6

PHZ 3151

Due Monday April 13

Please submit your code and plots wherever requested. Results can be handed in either as a hardcopy, or as an electronic document (e.g. tex, latex, MS word, or even a .pdf) sent via email.

1. In class, we discussed the diffusion equation and also a bit about Boltzmann statistics. In this problem, we will explore diffusion in the presence of an external field.

We saw in class that the mass current J_z of diffusing particles is given in terms of the diffusion constant D and local density $n(z, t)$ as

$$J_z = -D \frac{\partial n}{\partial z}$$

(in one dimension). Consider now an external field acting so that the diffusing particles feel an external force with z-component $F_z = -\frac{dU}{dz}$, where $U(z)$ is the potential energy of a particle at z . If the force $F_z = F_0$ (i.e. a constant force independent of z), then the potential energy is (up to a constant) $U(z) = -F_0 z$.

With this added force, the mass current is taken to be

$$J_z = -D \frac{\partial n}{\partial z} + n \mu F_0$$

where μ is the *mobility*.

a) Consider the case where $J_z = 0$ (i.e. equilibrium). Recall first that in equilibrium, based on our discussion of Boltzmann statistics, that at temperature T we have $n(z) = n_0 e^{-U(z)/k_B T}$. Next, show that there is a relationship between μ and D ,

$$\mu = \frac{D}{k_B T}$$

which was first determined by Einstein. The answer is obvious based on dimensional considerations. What it says is that there is a relationship between diffusion and drift in the presence of an external field because both are controlled by stochastic interactions between the particles and the surrounding medium. As an example, consider charged particles in a fluid interacting with an external electric field.

b) Use the continuity equation $\frac{\partial n}{\partial t} + \frac{\partial J_z}{\partial z} = 0$ to obtain the one-dimensional Smoluchowski equation,

$$\frac{\partial n}{\partial t} = D \frac{\partial^2 n}{\partial z^2} + \mu F_0 \frac{\partial n}{\partial z}$$

which can be used to model the response of a fluid to external fields including the approach to equilibrium.

2. Write a code that computes the average of many generated random numbers. Also, create and plot a histogram with the frequency of random numbers in certain ranges between zero and one. Does the average come out to be close to $\frac{1}{2}$ if you generate enough numbers? Finally, does the distribution of numbers in your histogram look to be uniform? Include a histogram with your report.

3. For a random number sequence $I_1, I_2, I_3, \dots, I_N$, compute *correlations* between numbers in the sequence. For example, for neighboring numbers in the sequence, we compute,

$$G_1 = \frac{1}{N-1} \sum_{i=1}^{N-1} (I_i - \frac{1}{2})(I_{i+1} - \frac{1}{2})$$

where we are assuming that the average of the sequence is $\frac{1}{2}$. More generally, we can compute correlations j numbers apart in the sequence as,

$$G_j = \frac{1}{N-j} \sum_{i=1}^{N-j} (I_i - \frac{1}{2})(I_{i+j} - \frac{1}{2})$$

for a truly random sequence, if we generate a large enough sequence, each correlation function G_j should be zero. It may seem like we get lucky at the poker table for a few hands or even a whole night, but if you play long enough you'll find there are really no correlations! Can you determine whether the correlation functions are zero to within the expected statistical error? Consider functions up to $j = 4$.

3. Now write a short and simple code to estimate π in the following way. Imagine inscribing a circle of radius equal 1 inside a square with the length of a side equal 2. Now generate a large number of random points (x, y) inside the square. Count up the fraction of points (x, y) are inside the circle. The chance of the point being inside the circle is proportional to the area of the circle divided by the area of the square. Since the area of the circle is π for radius=1, you can compute π in this way. For 10^9 random points, the number I get from the code I wrote is $\pi = 3.14164$. Can you predict how the accuracy depends on the number of random points?

4. Write a code to perform a random walk *and* a self-avoiding random walk in three dimensions. Run the code for many iterations, corresponding to a large ensemble of trajectories. Determine in both cases $\langle r^2 \rangle$ as a function of time. Make a log-log plot of your results, and determine from a linear fit to the data, as described in class, the exponents ν . Verify that $\nu = 1/2$ for the random walk, and $\nu \approx 3/5$ for the self-avoiding random walk in three dimensions. The self-avoiding random walk is a model for a polymer chain.