Some exercises on diffusion

1. Consider a random walk in one dimension, i.e., a particle that in each time interval Δt takes a step Δx, right or left, with displacements drawn from a probability distribution $f(\Delta x)$. Here we will focus on statistics of the total displacement, $x(t) - x(0) = \sum_{i=1}^{n} \Delta x_i$, after n steps.

   (i) Write a program that implements such a random walk for the specific case of a Gaussian displacement distribution:
   $$f(\Delta x) = (2\pi\sigma^2)^{-1/2} e^{-\Delta x^2/2\sigma^2}.$$
   Take $\sigma = 1$, and collect statistics for trajectories of length $n = 10$, $n = 20$, $n = 30$, ..., $n = 100$. Plot the average displacement $\langle (x(t) - x(0)) \rangle$ and the mean squared displacement $\langle (x(t) - x(0))^2 \rangle$ as functions of n. You should find (and be able to show on paper) that the mean squared displacement grows linearly with time,
   $$\langle (x(t) - x(0))^2 \rangle = 2Dt,$$
   where $t = n\Delta t$. This relationship defines the diffusion coefficient D.

   (ii) In order to complete part (i), it is necessary to draw random samples from a Gaussian distribution. You may have found it convenient to use a library for this purpose, or you may have written your own Gaussian random number generator. Either way, describe the algorithm for generating such samples, and show mathematically that these samples are indeed Gaussian distributed. Most such algorithms begin with random samples drawn from a uniform distribution on the interval $[0, 1]$; you do not need to describe how that basic utility works.

   (iii) In the limit of small σ and Δt, the probability $p(x - x(0), t)$ of observing a total displacement $x - x(0)$ after time t obeys the differential equation
   $$\frac{\partial p}{\partial t} = D \frac{\partial^2 p}{\partial x^2}. \tag{1}$$
   Show that
   $$p(x - x(0), t) = (4\pi Dt)^{-1/2} e^{-(x-x(0))^2/4Dt}$$
   solves this diffusion equation. Compare this analytical solution with histograms collected from your simulations with $n = 10$, $n = 20, \ldots$. (To do so, you will need to work out the relationship between D, σ, and Δt.)

2. Now consider a random walk with a different set of boundary conditions. Specifically, imagine that the walker always begins at $x(0) = 0$ and dies once it leaves the interval $-1/2 < x < 1/2$.

   (i) Using simulations, calculate the probability $S(t)$ that the walker still survives (i.e., has not left the interval $[-\frac{1}{2}, \frac{1}{2}]$) after a time t. Make a plot of $S(t)$ vs. t (or, equivalently, vs. n).

   Your results should depend on the value of σ you use. Explain why, and describe what range of values is both practical and reliable for comparing with predictions of Eq. 1.

   (ii) Also using simulations, make histograms of the position of walkers that still survive at time t (for a few different values of t). Before plotting these histograms, make sketches of your expectations.

(iii) The absorbing boundary condition can be imposed in a continuous dynamics (i.e., Eq. 1) by requiring that $p(-1/2,t) = p(1/2,t) = 0$. These constraints are easily satisfied in a Fourier series solution for $p(x,t)$, by including only terms with appropriate symmetry:

$$p(x,t) = \sum_{j=1,3,5,\ldots}^{\infty} a_j(t) \cos(j\pi x) \tag{2}$$

Using the differential equation (1), together with the initial condition $a_j(0) = 2$, solve for the Fourier coefficients $a_j(t)$.

(iv) For a few values of t, compare your simulation results for $p(x,t)$ with the Fourier series determined in part(iii), calculated by numerically summing terms up to some manageable value of j.

(v) By integrating Eq. 2, write a Fourier series for the survival probability $S(t)$. Evaluate it numerically (again by summing terms up to some manageable value of j), and compare with your simulation results.