PHY2108 Stochastic Processes. Homework 2

Problem 1. Transcription factor (TF) slides on the DNA, starting at some position x_0. At each time step, it moves one step forward with a probability p or moves backward with a probability q. Once it reaches a specific location $x_f > x_0$ to which it binds very weakly ("stop" sequence), it falls off.

1.1 What is the probability that it will never fall off in either case (as a function of x_0)? Consider both cases when $p > q$ and $p < q$. You can use either full discrete form or the Fokker Planck approximation.

1.2 For $p > q$, calculate the average time it will take the TF to fall off the DNA, as a function of the original distance from the "stop" sequence. What happens to this time when $p \to q$? Why? You ca+n use either full discrete form or the Fokker Planck approximation.

1.3 Simulate the process to confirm your calculations in **1.1** and **1.2**.

1.4 (*Bonus*) Show that the discrete and FP results they become equivalent when $|p - q| \ll 1$.

Problem 2. A molecule can decay via two different independent processes. The probability to decay via the first process in a time interval dt is $r_1 dt$ and via the second process is $r_2 dt$.

2.1 Write the equation for $S(t)$ - the probability that the molecule still has not decayed by time t.

2.2 Calculate the probability that after waiting for a very long (infinite) time the molecule has decayed via the first process.

2.3 Calculate the mean conditional decay times via either of the processes. What are the probability distributions of these times?

2.3 Verify the theoretical predictions using Gillespie algorithm

Problem 3: Langevin equation and Smolluchowski equation. A molecule consists of two atoms separated by a distance r. The atoms are connected by a bond that can be approximated by a harmonic spring, so that its energy as a function of the separation between the atoms is $U(r) = ak_BTr^2/2$.

3.1 Write the Somluchowski equation for the probability $P(r, t)$ for the atoms to be at a distance r from each other. (You can assume that the atoms can pass through each other, and there is no steric repulsion between them). What is the steady state (equilibrium) distribution $P(r)^{\text{eq}}$? Can you find the dynamical solution $P(r, t)$?

3.1 Write the Langevin equation for the interatomic distance r. Calculate the mean r and center of mass and its variance as a function of time.

3.2 Simulate the Langevin dynamics and verify that it agrees with the theoretical calculations.

Problem 4.(Bonus 10 pt) First passage in higher dimensions. A molecule is diffusing near a spherical surface of radius a, starting at the initial distance from the origin $r > a$. When it gets to the surface, it binds it and is never released. On the other hand, when it gets to distance b from the origin, it is absorbed and disappears.

4.1 Using the appropriate backward equations in spherical coordinates with appropriate boundary condition and calculate the probability and the average time to at the surface at a. You can assume that it is radially symmetric.

4.2 Calculate the average time to reach either one of the surfaces.

4.3 What happens to this time when $a \to 0$? $b \to \infty$?

Each problem has equal weight.

Problem 5. . A fluorophore molecule can be in two states: fluorescent (1) and non-fluorescent (2). The transition rate between the two states (in both directions) is r. From either state, the molecule can transition to a long lived refractory state, from which it never recovers on the time scale of the experiment, with a rate r_o.

5.1 Write the Master equation for the molecule. Calculate the probability that it is still not in the refractory state at time t, assuming it starts in the non-fluorescent state.

5.2 Calculate the mean time till it becomes refractory. Calculate the mean time the molecule is fluorescent before it goes refractory. Calculate the variances of these times.