CH163: HW3
Due 9/29/2022 at 9 am

Problem 1)

X and Y are independent random variables obeying Poisson statistics with parameters μ and ν:

$$P(X=n)=\frac{e^{-\mu}\mu^n}{n!} \quad and \quad P(Y=n)=\frac{e^{-\nu}\nu^n}{n!} \quad n=0,1,2\ldots$$

(a) Prove that (X+Y) obeys Poission statistics with parameter $(\mu+\nu)$:

$$P(X+Y=n)=\frac{e^{-(\mu+\nu)}(\mu+\nu)^n}{n!} \quad n=0,1,2\ldots$$

Hint: exploit the binomial formula: $$(\mu+\nu)^n=\sum_{k=0}^{n}\frac{n!}{k!(n-k)!}\mu^k\nu^{n-k}$$

(b) Suppose you have two continuous light sources, one of which delivers, on average μ photons/s and the other delivers ν photons/s. You shine both light sources simultaneously on a photon-counting detector. What is the probability distribution for the number of photon counts detected per second?

(c) Now suppose that the detector only has a 50% Quantum Yield (this means that it only has a 50% probability of registering a photon that strikes it. What is the probability distribution for the number of photon counts detected per second?

Problem 2)

(a) Read the paper: "Kinesin Moves by an Asymmetric Hand-Over-Hand Mechanism" [C. L. Asbury, A. N. Fehr, and S. M. Block, *Science,* **302**, 2130 (2003).] Kinesin always takes 8 nm steps, but these authors showed that under a 4 pN rearward load, the DmK401 mutant has different characteristic dwell times for even and odd numbered steps. Dwell times were distributed nearly exponentially, but with characteristic lifetimes that alternated between 136 ms and 24 ms. In this problem we will build a model for the motion of this kinesin mutant over times long compared to the step time.

The walk of a kinesin molecule is a bit different from a regular random walk because the step size is fixed (8 nm), but the step *time* is random. Normally we think of the time of steps as occurring in regular intervals and the distances as being random.

(b) First let's suppose that all the steps are sampled from the same exponential distribution of dwell times with mean dwell time τ. Write down this single-step probability distribution, $P_1(t)$, its mean, and its variance. The probability distribution $P(N)$ for the number N of steps in time t is Poisson distributed (each step is statistically akin to a single decay event in a radioactive sample). Write down $P(N)$ in terms of t and τ. For large t, $P(N)$ starts to look like a Gaussian distribution (with N now acting as a continuous variable). Write down the Gaussian approximation to $P(N)$. Hint: match the mean and variance to the Poisson distribution.

(c) Calculate the probability distribution of the time t that it takes to go N steps, where N is large. You can find this time by applying the Central Limit Theorem to the time distribution for a single step. Now let's put back the requirement that we alternate fast steps, with time constant τ_F and slow steps with time constant τ_S. This means we take $N/2$ fast steps and $N/2$ slow steps. What is the probability distribution for the total time to take all of these steps? What is the average time to go N steps?

Problem 3)

Consider a spherical Brownian particle of radius a, density ρ, in a medium of viscosity η, bound by a harmonic potential, $U(x) = \frac{1}{2} k x^2$.

(a) What is the momentum relaxation time for the particle?
(b) Assuming that the motion is overdamped, what is the relaxation time due to the confining potential?
(c) Establish the relationship between a, ρ, and η for which the momentum relaxation time for the free particle equals the drift relaxation time for overdamped motion in the potential. This balance determines whether the motion of a particle is overdamped or underdamped.
(d) If you decrease a, keeping all else constant, does the effect of damping increase or decrease?

Problem 4)

Howard problem 4.7: If a particle is confined by a potential $U(x) = F|x|$, that is, a particle is trapped between two linear inclines, show that $\langle U \rangle = k_B T$ (and not $\frac{1}{2} k_B T$). Is this or isn't this a violation of the Equipartition Theorem?

Problem 5)

Ladislaus von Bortkewitsch (1868-1931) was a Russian statistician who popularized the Poisson distribution. He studied data on death by horse kick in the Prussian military, which we can assume are low probability and statistically independent events. He examined 14 Corps over 20 years (280 samples total) and tallied the frequency of each number of deaths. A summary of his data is in the table below:

Deaths by horse kick	# of occurrences
0	144
1	91
2	32
3	11
4	2
5+	0
Total	**280**

Type this data into Matlab and fit it to a Poisson distribution with parameter **`lambda`**. You can perform the fit using the same approach as the fitting on last week's homework. Hint: the function **`poisspdf`** will give you a Poisson distribution. What is **`lambda`**? Submit a plot showing the probability distribution and the Poisson fit. What was the probability of having 10 deaths by horse kick in one unit of the Prussian army in one year?

Problem 6)
Simulation of a Brownian ratchet
In this problem you will write a MATLAB program to simulate the motion of a particle obeying an overdamped Langevin equation of motion in an arbitrary 1-D potential. You will check that the particle obeys the Boltzmann distribution and Equipartition.

This program can be used to simulate the motion of a molecular motor on a microtubule, a protein sliding along DNA, a bead in an optical trap, the unzipping of a piece of DNA, or the unfolding of a protein by an external force.

Recall from class, the equation of motion of an overdamped particle subject to an external force:

$$\frac{dx}{dt} = \frac{F}{\gamma} + \frac{\xi(t)}{\gamma}, \qquad [1]$$

where F is the force, γ is the drag coefficient, and ξ is Gaussian distributed white-noise with mean 0 and autocorrelation

$$\langle \xi(t)\xi(0) \rangle = 2k_B T\gamma\delta(t)$$

To run a simulation we need a discrete-time version of Eq. 1. We obtain this equation by integrating Eq. 1 from time t to $t + \Delta t$. Then we get:

$$x(t+\Delta t) = x(t) + \frac{F}{\gamma}\Delta t + \sqrt{2D\Delta t}\,N(0,1), \quad [2]$$

where $N(0,1)$ is a Gaussian random variable with mean 0 and variance 1.

1) Write a MATLAB program with the following header:

```
function out = Langevin(D, dt, nsteps, T, x0, X, U)
% function out = Langevin(D, dt, nsteps, T, x0, X, U)
% D = diffusion coefficient (m^2/s)
% dt = time step (s)
% nsteps = # of steps to simulate
% T = absolute temperature
% x0 = starting position (m)
% X = vector of positions at which the potential is given (m)
% U = vector containing the potential (J)
```

The program should simulate a Brownian trajectory according to Eq. 2.
Some functions that might be useful in doing this are:

```
gradient
randn
```

To time how long your program takes to run, you can use the `tic` and `toc` commands, which return the time elapsed between calling `tic` and calling `toc`. For instance, you might write:

```
tic;
trajec = Langevin(D, dt, nsteps, T, x0, X, U);
toc
```

This can be useful in trying to find ways to make your code run faster. One version of this program took 0.07 seconds to run a trajectory of 100,000 steps on a PC.

2) Write a script to simulate motion in a harmonic well.

a) Run a simulation with the following conditions:

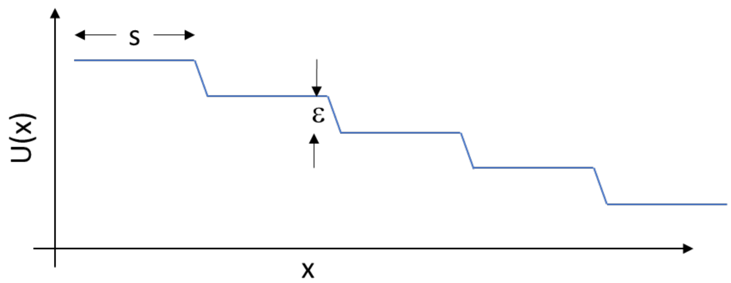
***D* = 10^{-10} m^2/s**: This corresponds to a ~4 nm diameter particle in water.
dt = 10^{-3} s
nsteps = 100000: This corresponds to 100 s of data.
T = 298 K: Room temperature.
x0 = 0
X = (-1000:1000)*1e-8: This corresponds to a field of view from -10 μm to 10 μm.
U = ½ k x^2: Try k = 3 x 10^{-9} N/m.

b) Submit a plot of *U*(*x*) in units of k_BT, and on the same axis a histogram of the probability distribution for *x*. You can scale the amplitude of the probability distribution to give it approximately the same scale as *U*(*x*).

c) Calculate the mean potential energy of the particle from your trajectory. Compare this energy to k_BT. Is the Equipartition Theorem satisfied?

3) Write a script to simulate a Brownian ratchet.

a) You can implement the nearly irreversible binding that occurs when the ratchet crosses a threshold by putting steep drops into your potential. These effectively implement a ratchet:



Design a ratchet potential with:

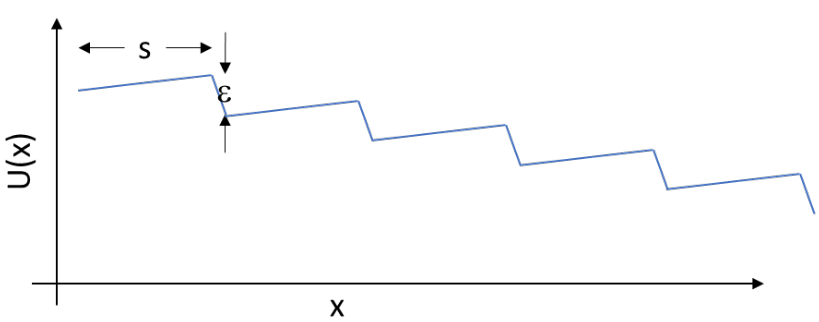
S = 8 nm: matched to the step size of kinesin
ε = 5 k_BT: a relatively weak binding interaction, but still strong enough that backward steps are rare.
Connect the flat parts of the potential by linear ramps over 1 nm.

***D* = 10^{-10} m^2/s**: This corresponds to a ~4 nm diameter particle in water.
dt = 10^{-9} s
nsteps = 100000: This corresponds to 100 microseconds of simulation time
T = 298 K: Room temperature.
x0 = 0
X = (-200:2000)*1e-10: This corresponds to a field of view from -20 nm to 200 nm.

b) Run the simulation enough times to estimate the average velocity of the particle.

c) Cut *s* in half, to 4 nm. What does this do to the velocity? Is this consistent with your expectations from class?

d) Using *s* = 8 nm, now see how this molecular motor performs against an opposing force. Then the potential would look something like this:



Construct a potential where the opposing force is 0.5 pN. Make a plot of the potential. What is the average velocity?

e) Calculate a force-velocity curve for this motor. Consider the following force values (all in pN): -1, -0.5, 0, 0.5, 1, 2. Here a negative force means the force is assisting the motor. Make a plot of $\langle v \rangle$ vs. F. Can you predict what the stall force of the motor will be? Is it possible to force the motor to run backward?