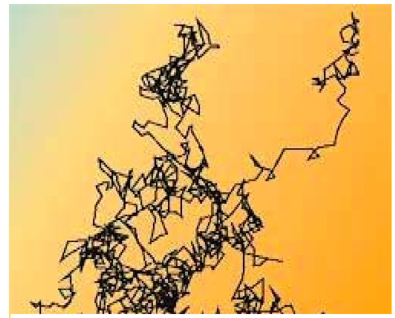
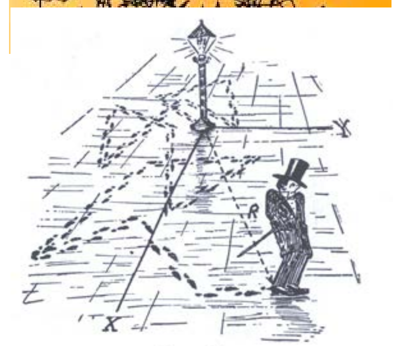
1D Diffusion





***Central Question*:**

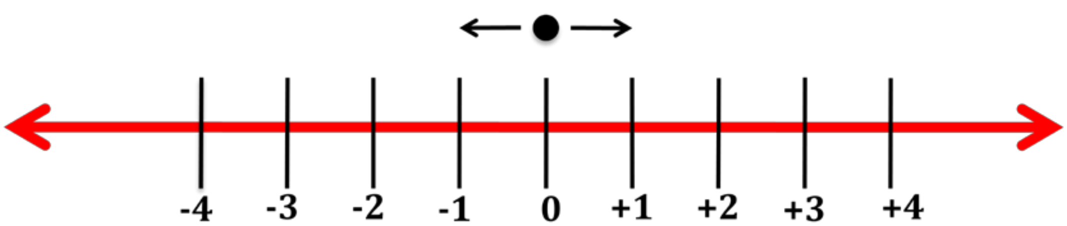
Most of us have the intuition that a group of molecules located in the center of a room will spontaneously diffuse from their starting position until eventually they are distributed throughout the space that they have available to them.

But why does this happen? *How can we show that it is more likely for the molecules to spread out than to remain bunched up in the center of the room? That's what we will try to answer in this recitation.*

Part I. Following a Single Molecule

Let's explore what happens to a molecule that is jostled randomly by neighboring molecules in a cellular environment. Imagine that we have a whole bunch of molecules, but that we are able to paint a black dot on one of them, and follow this black-dotted molecule around.

Suppose for simplicity that such a black-dotted molecule is located at $x = 0$ and confined to move along one dimension. Let's call that dimension the x-axis (see Figure below). Because this molecule experiences random collisions with nearby molecules, it has an equal chance of moving a step to the left to $x = -1$, moving a step to the right to $x = +1$, or staying put at $x = 0$. The probability of each of these events happening is 1/3. Each step that the molecule takes obeys these rules.



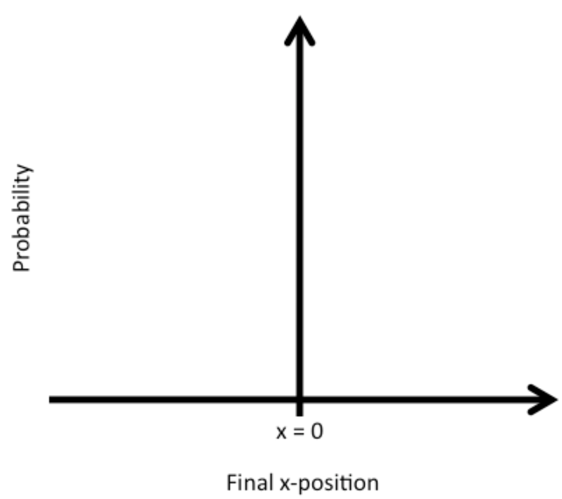
Prompt 1. After the molecule undergoes <u>2 steps</u>, determine the probability that it ends up at (a) $x = 0$, (b) $x = +1$, (c) $x = -1$, (d) $x = +2$, and (e) $x = -2$.

Prompt 2. After the molecule undergoes <u>3 steps</u>, determine the probability that it ends up at (a) $x = 0$, (b) $x = +1$, (c) $x = -1$, (d) $x = +2$, and (e) $x = -2$.

Prompt 3. Fill in the following table. For each final position, determine how many possible paths the molecule could take to get there given a particular number of steps.

Final Position	Number of Possible Paths			
	1 step	2 steps	3 steps	4 steps
x = +4				
x = +3				
x = +2				
x = +1				
x = 0				
x = -1				
x = -2				
x = -3				
x = -4				

Prompt 4. Plot the <u>probability</u> (you can use Excel if you like, or just sketch the plots by hand) of a molecule arriving at a particular position along the *x*-axis after *N* steps (axes for these plots shown below), where *N* = 1, 2, 3, and 4. That is, create four plots on the same set of axes (one for *N* = 1, one for *N* = 2, one for *N* = 3, and one for *N* = 4). Label each plot with its *N* value.



Prompt 5. Use your plots to describe what happens to the probability of finding the molecule at different positions along the *x*-axis as the number of steps increases. What would happen as the number of steps *N* got really large?

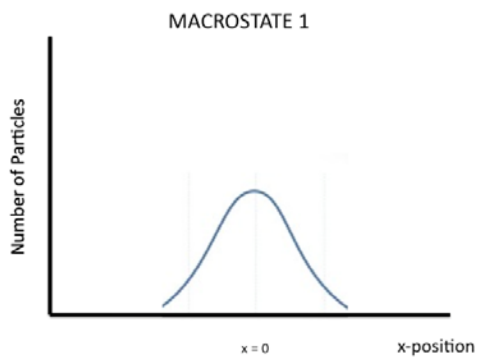
Prompt 6. Why is the probability of finding the molecule at *x* = 0 greater than the probability of finding the molecule at some other value of *x*, after any number of steps *N*?

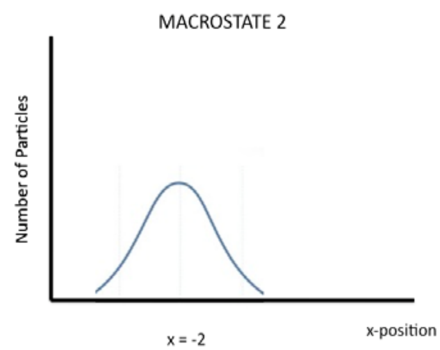
Part II. Many Particles: Microstates, Macrostates, and Entropy

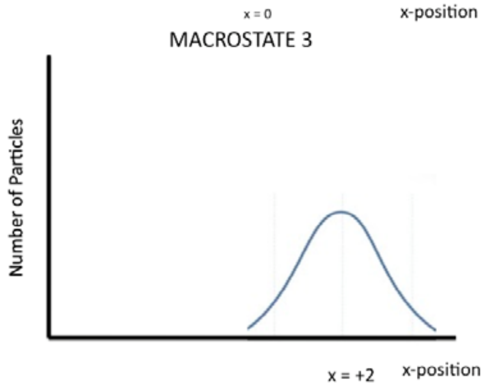
The assumption in Part I was that we were following around a single molecule as it was jostled by nearby molecules. Now let's consider what would happen if we had a system consisting of a LOT of identical molecules located initially at x = 0, each undergoing 1D random walks. Suppose we could follow all of them.

In this scenario, a *microstate* of the system specifies the particular position on the x-axis of every single particle at a particular time. A *macrostate* of the system specifies only *how many* particles end up at each position along the x-axis at a particular time (say, 4 particles at x = -1, 3 particles at x = 0, 7 particles at x = +1, etc) but does not specify *which* specific particles end up where. *Make sure you understand this distinction*! A particular <u>macrostate</u> can be represented by a plot showing how many particles exist at each position along the x-axis at a particular time t.

Three example macrostates for this system (all particles at x = 0 at t = 0) are shown here for some time t:







Prompt 7. Rank the macrostates shown above from the most probable to the least probable. *Use what you found in Part I of this recitation to justify your ranking in terms of the number of microstates associated with each macrostate*.

Prompt 8. Suppose that the system is in MACROSTATE 1 (shown above) at some initial time t. Explain why the curve representing the system's macrostate flattens and spreads as time goes on.

Prompt 9. Entropy is a measure of the number of microstates associated with a particular macrostate. Explain, using microstate and macrostate language, why the diffusion of particles away from their initial position at x = 0 is accompanied by an increase in the entropy of the system.