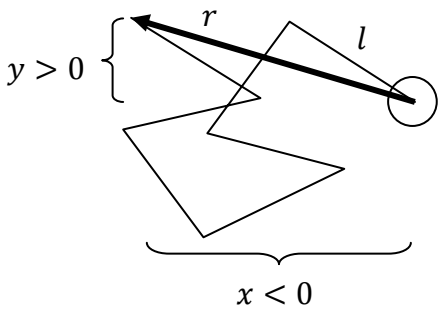
Handout 5
Random Walks

Consider a sea of molecules. Pinpoint one molecule and note its starting position at time 0. Let this position define the coordinate origin. We will assume that, due to thermal motion, the particle on average makes a random jump of length l every τ units of time. The jump is random in the radial direction. This is called a **random walk**.

One could imagine the particle experiencing a very large number of jumps. We might interrogate the final position of the particle after n such jumps.



We could imagine performing many such experiments for the same particle, each time starting at the same location but with a different series of random jumps. What would be the expected $\langle x \rangle$, $\langle y \rangle$, $\langle z \rangle$ after n jumps if we averaged over all of these experiments? Some of the experiments will end up with positive x, while some negative, and similarly for the y and z directions. Since the particle has no bias to go in the positive or negative direction, the averages over the experiments must be

$$\langle x \rangle = 0 \quad \langle y \rangle = 0 \quad \langle z \rangle = 0$$

On the other hand, we can ask how far the particle has traveled in absolute distance from its initial location. Let r_n be the distance traveled after n steps. Note that r_n is always a positive number, since it is a distance and not a coordinate. We will compute the average squared distance $\langle r_n^2 \rangle$ over all possible experiments. We begin by noting that

$$r_n^2 = x_n^2 + y_n^2 + z_n^2$$

Consider the case in going from step n to $n+1$:

$$\begin{aligned} r_{n+1}^2 - r_n^2 &= x_{n+1}^2 - x_n^2 + y_{n+1}^2 - y_n^2 + z_{n+1}^2 - z_n^2 \\ &= (x_n + \Delta x)^2 - x_n^2 + (y_n + \Delta \mathrm{y})^2 - y_n^2 + (z_n + \Delta z)^2 - z_n^2 \\ &= (x_n + \Delta x)^2 - x_n^2 + (y_n + \Delta \mathrm{y})^2 - y_n^2 + (z_n + \Delta z)^2 - z_n^2 \end{aligned}$$

$$= 2x_n\Delta x + \Delta x^2 + 2y_n\Delta y + \Delta y^2 + 2z_n\Delta z + \Delta z^2$$

Here, $\Delta x, \Delta y, \Delta z$ are the random amounts by which we change the length at one step. Notice that we have the constraint $\Delta x^2 + \Delta y^2 + \Delta z^2 = l^2$ because these random amounts must add up to give the length of one jump. Therefore

$$r_{n+1}^2 - r_n^2 = 2x_n\Delta x + 2y_n\Delta y + 2z_n\Delta z + l^2$$

Now, we average over all possible (random) trajectories for the same starting point:

$$\langle r_{n+1}^2 - r_n^2 \rangle = \langle 2x_n\Delta x + 2y_n\Delta y + 2z_n\Delta z \rangle + l^2$$

However, $\Delta x, \Delta y, \Delta z$ are random at each step and they are completely uncorrelated with the position of the molecule. That is, the amount of the random jump in the x direction, Δx, is unaffected by the x position of the molecule. Thus,

$$\langle r_{n+1}^2 - r_n^2 \rangle = 2\langle x_n \rangle\langle \Delta x \rangle + 2\langle y_n \rangle\langle \Delta y \rangle + 2\langle z_n \rangle\langle \Delta z \rangle + l^2$$

But the averages of $\Delta x, \Delta y, \Delta z$ and of x, y, z are all zero, since the random walk has no net direction. Thus, we obtain

$$\langle r_{n+1}^2 - r_n^2 \rangle = l^2$$

Or

$$\langle r_{n+1}^2 \rangle = \langle r_n^2 \rangle + l^2$$

Starting at $n = 0$,

$$\langle r_0^2 \rangle = 0 \qquad \langle r_1^2 \rangle = l^2 \qquad \langle r_2^2 \rangle = 2l^2 \quad \ldots$$

By recursion, therefore, we can write

$$\begin{aligned} \langle r_n^2 \rangle &= nl^2 \\ &= \frac{t}{\tau} l^2 \end{aligned}$$

The LHS is called the **mean squared displacement**. It tracks the average squared distance of a particle at its random location at time t from its initial location. This kind of random movement is called **Brownian motion** and is a kind of **diffusive** process. Here, diffusive means that the motion is dominated by random fluctuations. In fact, we can define the diffusion constant using the above model,

$$D \equiv \frac{l^2}{6\tau}$$

with

$$\langle r^2 \rangle = 6Dt$$