Lecture 30x – Random walks (extended version)

Many aspects of mechanics that have been discussed so far in this course are deterministic, in the sense that from a given initial condition (say an initial position and velocity) classical mechanics predicts exactly what trajectory an object follows as a function of time. Now, we turn to systems where individual trajectories may be difficult to follow for a variety of reasons – for example, there may be a whole collection of objects interacting with each other, and thus influencing their individual motion. Although we might despair of analyzing such systems, they may have colllective properties that can be described mathematically and obey compact physical laws. For example, we don't need to know the inidivdual trajectories of molecules in a gas to understand the ideal gas law, which relates the pressure of a gas to its volume or temperature throughy $PV = nRT$. In general, this part of mechanics is called *statistical mechanics* and it describes the properties of a system when averaged over:

- the many particles in a system, or
- many non-identical copies of a system, or
- the time history of a system.

Most students have already run across this concept when they were first introduced to the atomic orbitals of quantum mechanics. There, the orbital doesn't give the exact location of an electron, but rather the likelihood of finding an electron at a particular location. Why this approach is so important to biological materials is because they are soft, in the sense that they are easy to deform, or they flop around at room temperature. Some biological systems are soft even compared to a gas; for example, we've already discussed the very small compression resistance of the spectrin network of the red blood cell.

A discussion of statistical mechanics often starts with the behaviour of the so-called *random walk*. An anthropometric example of a random walk is the trajectory of a drunken sailor, to use a slightly derogatory description of sailors. We imagine the sailor starts off a lamppost at night and, being drunk, disoriented and walking in the dark, cannot see where he is going. He takes N steps, probably of slightly different length and certainly of varying direction. Now, if he were sober and walking along a street in the daylight, the length of his path would be N times the length of each step. At night, the distance that he walks is still governed by this rule (sum over the lengths of each step), but the end-to-end displacement of his trajectory is much less. That is, if each step has the same length b, then

$[distance] = Nb$ (sober or drunk, its just the path length)

but

$[displacement] \sim Nb$ (sober, straight line)
$[displacement\} << Nb$ (random directions).

It's probably unfair to use a nineteenth century stereotype of sailors as an illustration, but one could also imagine random walks to be taken by animals and insects looking for food: a straight trajectory is followed for a short time and, if no food is found, the trajectory is randomly changed to a different direction.

Now, let's describe the random walk mathematically. Characterize each step of the walk by a vector $\mathbf{b}_i$, which has a magnitude and direction. The *distance* or contour length of the path, is the just the scalar sum over the individual steps:

[*contour length*] = $L = \Sigma_{i=1,N}\, b_i$. (1)

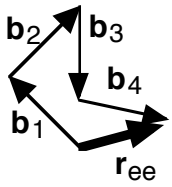
Eq. (1) is a scalar equation – it is just a sum over the (scalar) lengths of each step. There is no direction dependence to Eq. (1) so that no matter how the path twists and turns, the contour length is always the same if the average step size is the same.

It's a different story for the displacement of the path, which is the distance from the start point to the stop point. Here, the end-to-end displacement is represented by the **vector** $\mathbf{r}_{ee}$. In the diagram below, it's easy to see that

$L = b_1 + b_2 + b_3 + b_4$ all scalars

whereas

$\mathbf{r}_{ee} = \mathbf{b}_1 + \mathbf{b}_2 + \mathbf{b}_3 + \mathbf{b}_4$ all vectors



For this walk, the magnitude of the displace r_{ee} is much less than L. For N steps, the summation for the displacement is:

$\mathbf{r}_{ee} = \Sigma_{i=1,N}\, \mathbf{b}_i$. (2)

Demo: In class, we construct random walks with a series of plastic vectors (strips of rigid white plastic that are 1" wide and 1' long, to use imperial units) each of which has the same length which we define as B. It doesn't matter what the particular size of B is. The "tip" of each vector is marked with coloured tape, one colour for each ten vectors. A vector is thrown randomly into the air, and, once it hits the floor, it is translated by hand *without rotation* so that its tail is placed on the tip of the previous vector. After 10 vectors have been joined together to form a single random walk, the end-to-end displacement $\mathbf{r}_{ee}$ is measured with a tape measure. All walks have the same contour length $L = 10B$ according to Eq. (1). A set of measurements from class is:

Trial	r_{ee}	L
1	5.5B	10B
2	2.5B	10B
3	0.8B	10B
4	0.5B	10B
5	4.5B	10B
6	4.2B	10B
7	5.6B	10B
8	3.0B	10B

The data immediately show two things:
•the magnitude of $\mathbf{r}_{ee}$ is barely more than 50% of L at the best, and is often much less
•there is a range of values of r_{ee}.

From the data, we now construct the mean value of $\mathbf{r}_{ee}^2$. Why square this? Because it's a vector and, properly speaking, the length of a vector is found from the dot product of the vector with itself:

$$\mathbf{r}_{ee}^2 = \mathbf{r}_{ee} \cdot \mathbf{r}_{ee} = \textit{magnitude of displacement}^2 = r_{ee}^2.$$

Yes, this equation looks trivial, but it says that the scalar length squared of a vector is equal to the (scalar) dot product of a vector with itself. The data show that

$$\langle \mathbf{r}_{ee}^2 \rangle = (5.5^2 + 2.5^2 + 0.8^2 + 0.5^2 + 4.5^2 + 4.2^2 + 5.6^2 + 3.0^2)\, B^2 / 8$$
$$= 14.5\, B^2. \qquad (3)$$

The notation < … > means "take the average". Notice just how small $\langle \mathbf{r}_{ee}^2 \rangle$ is compared to

$$L^2 = 100\, B^2 \qquad \text{(same for all walks)}$$

[*end of demo*]

Random walks with equal steps

Even though each individual value of $\mathbf{r}_{ee}^2$ is different, it turns out that it is very easy to calculate the average value of $\mathbf{r}_{ee}^2$ when taken over a large number of different configurations. For now, each step is assumed to have the same unit length b, even though the directions are different from step to step. From Eq. (2), the general form of the dot product of $\mathbf{r}_{ee}$ with itself for a particular walk is

$$\mathbf{r}_{ee} \cdot \mathbf{r}_{ee} = (\Sigma_{i=1,N}\, \mathbf{b}_i) \cdot (\Sigma_{i=1,N}\, \mathbf{b}_i)$$

$$= (\mathbf{b}_1 + \mathbf{b}_2 + \mathbf{b}_3 + ...) \cdot (\mathbf{b}_1 + \mathbf{b}_2 + \mathbf{b}_3 + ...)$$

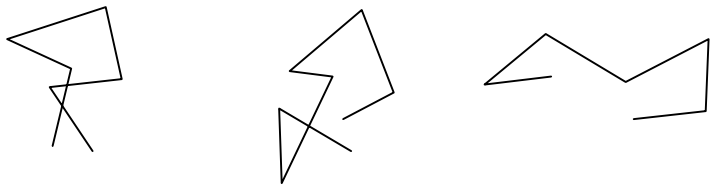
$$= \mathbf{b}_1^2 + \mathbf{b}_2^2 + \mathbf{b}_3^2 \ldots + 2\mathbf{b}_1 \cdot \mathbf{b}_2 + 2\mathbf{b}_1 \cdot \mathbf{b}_3 + 2\mathbf{b}_1 \cdot \mathbf{b}_4 + \ldots + 2\mathbf{b}_2 \cdot \mathbf{b}_3 .... \qquad (4)$$

Each of the terms in this sum is a scalar. There are N terms of the form $\mathbf{b}_i^2$, each of

which is just b^2, since all steps have the same length. Thus, for a given walk

$$\mathbf{r}_{ee}^{\,2} = Nb^2 + 2\mathbf{b}_1\cdot\mathbf{b}_2 + 2\mathbf{b}_1\cdot\mathbf{b}_3 + 2\mathbf{b}_1\cdot\mathbf{b}_4 + \ldots + 2\mathbf{b}_2\cdot\mathbf{b}_3\ldots. \qquad (5)$$

Now, we generate $\mathbf{r}_{ee}$ for a given chain with Eq. (5). But there are an infinite number of random walks of N steps starting from the same origin:



We find the average value $\langle \mathbf{r}_{ee}^{\,2} \rangle$ by summing over all these paths. At first, this looks intimidating, but the mathematics is actually quite simple. From Eq. (5), the mean value $\langle \mathbf{r}_{ee}^{\,2} \rangle$ is:

$$\langle \mathbf{r}_{ee}^{\,2} \rangle = Nb^2 + 2(\mathbf{b}_1\cdot\mathbf{b}_2)_{av} + 2(\mathbf{b}_1\cdot\mathbf{b}_3)_{av} + 2(\mathbf{b}_1\cdot\mathbf{b}_4)_{av} + \ldots + 2(\mathbf{b}_2\cdot\mathbf{b}_3)_{av}\ldots. \qquad (6)$$

where $(\ldots)_{av}$ and $\langle \ldots \rangle$ mean "construct the average".

The average value of $\mathbf{b}_1\cdot\mathbf{b}_2$ is the average dot product of $\mathbf{b}_1$ with all other vectors $\mathbf{b}_2$ from all the different paths. Some $\mathbf{b}_2$'s point in the same direction as $\mathbf{b}_1$ and some point in the opposite direction:

$\mathbf{b}_1\cdot\mathbf{b}_2 = b^2$ if $\mathbf{b}_1$ and $\mathbf{b}_2$ point in exactly the same direction
$\mathbf{b}_1\cdot\mathbf{b}_2 = -b^2$ if $\mathbf{b}_1$ and $\mathbf{b}_2$ point in exactly the opposite direction

The bottom line is that for every configuration with a particular scalar value $\mathbf{b}_1\cdot\mathbf{b}_2 = b_{12}$, there is another configuration with $\mathbf{b}_1\cdot\mathbf{b}_2 = -b_{12}$, because the orientations are completely random. Thus, averaged over all possible configurations

$$(\mathbf{b}_1\cdot\mathbf{b}_2)_{av} = 0. \qquad (7)$$

The same goes for all other combinations, as long as the indices are different. So, we find the simple, elegant and **very important** result

$$\langle \mathbf{r}_{ee}^{\,2} \rangle = Nb^2. \qquad \text{(random walk)} \qquad (8)$$

Recalling that the contour length L is equal to

$$L = Nb$$

then another way of writing $\langle \mathbf{r}_{ee}^{\,2} \rangle$ is

$$\langle \mathbf{r}_{ee}^{\,2} \rangle = bL. \qquad \text{(random walk)} \qquad (9)$$

Returning to our in-class demo of $N = 10$ steps each of length B, Eq. (8) predicts that

$$\langle \mathbf{r}_{ee}^{\,2} \rangle = 10B^2 \qquad \text{(demo)}$$

The measured data give $\langle \mathbf{r}_{ee}^2 \rangle = 14B^2$, which is in not bad agreement considering the nature of the experiment. Certainly, we did *not* observe $\langle \mathbf{r}_{ee}^2 \rangle = 100B^2$ expected for straight lines.

Example: proteins

A protein is a linear sequence of amino acids, of which 20 types are found in the proteins in our bodies. Each contributes 0.36 nm to the contour length of the string

AA — AA — AA — AA — AA

For example, the protein actin, a major part of our muscles, is 375 AA long, giving an overall length of about 135 nm. But the amino acid backbone of a protein does not behave like a stiff rod; rather, it wiggles and sticks to itself at various locations. The random walk gives an approximate value for its size (a better calculation would include self-interactions along the protein chain):

$$\langle \mathbf{r}_{ee}^2 \rangle = Nb^2 = 375\ (0.36)^2$$

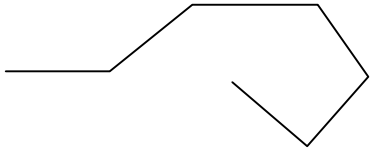
or

$$r_{ee,av} \sim \sqrt{375} \times 0.36 = 7.0 \text{ nm}$$

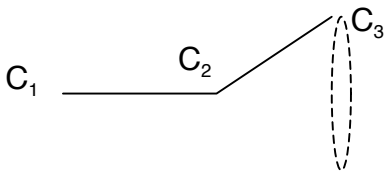
In other words, the radius of a random ball of actin (<10 nm) is *much* less than its length when fully stretched (135 nm).

Persistence length

The calculation above was for a freely-jointed chain – any angular orientation of the joint has the same energy. What happens if this is not true: suppose that a strong deformation requires more energy than a mild deformation? As an example, consider the configurations of a saturated alkane, $-CH_2-$ (repeated), where the polar angle between successive carbons is close to the tetrahedral value of 109.5°, but the chain is free to rotate in the azimuthal angle about the C-C bond.



That is, for a particular carbon-carbon bond C_1-C_2, the polar angle of the bond C_2-C_3 is fixed, but C_3 is free to rotate azimuthally about the C_1-C_2 axis:



One can show that the general behaviour of the ideal chain $\langle r_{ee}^2 \rangle \sim N$ still holds, but the prefactor in the scaling law is different. If the polar angle C_1-C_2-C_3 is fixed at α, then

$$\langle r_{ee}^2 \rangle = Nb^2 (1 - \cos\alpha) / (1 + \cos\alpha) \quad (10)$$

where b is the bond length. Using $\alpha = 109.5^o$,

$$(1 - \cos\alpha) / (1 + \cos\alpha) = (4/3) / (2/3) = 2$$

Thus, in this case

$$\langle r_{ee}^2 \rangle = 2Nb^2 = (2b)(Nb) = (2b) L \quad (11)$$

where L is the total length of the chain, $L = Nb$. Eq. (10) is referred to as the freely-rotating chain, in contrast to the freely-jointed chain that is the analogue of the random walk.

What can we conclude by comparing Eqs. (9) and (11):

First, the scaling of $\langle r_{ee}^2 \rangle$ with L in Eq. (11) is the same as a freely jointed chain Eq. (9); however, $\langle r_{ee}^2 \rangle$ is now larger by a factor of two because the chain is effectively stiffer.

Second, this suggests a way of parametrizing the stiffness of the chain through the introduction of a persistence length ξ in

$$\langle r_{ee}^2 \rangle = 2\xi L \quad (12)$$

In the above examples:

Freely jointed chain $\xi = b / 2$

Alkane model $\xi = b$.

The physical interpretation of the persistence length is that it measures the minimum length scale along which a filament fluctuates in direction. The stiffer the filament, the longer the "wavelength" of the deformation on the filament, and as a result, the larger ξ is.

Biological examples

A biological cell may contain a variety of filament of different thickness and stiffness. Some common examples are

Filament	ξ (nm)
Alkane	0.5
DNA	53
filamentous actin	10-20 x 10^3
microtubules	1-6 x 10^6

Note that ξ of the cell's filaments span an enormous range. How do they do that - does

the variation in stiffness mean that a microtubule is a million times the diameter of the DNA double helix? The answer is "no" and the reason is that the persistence length of a uniform rod grows like the fourth power of its radius. Thus, doubling the radius of a rod increases it persistence length by a factor of $2^4 = 16$.

A simple calculation of $\langle r_{ee}^2 \rangle$ for DNA with a persistence length of 53 nm shows that bacterial DNA is balled up into a region roughly the size of a bacterium, but human DNA is too large to fit into a normal eucaryotic cell, let alone its nucleus. This calculation is left to the student as a problem set. The fact that human DNA doesn't fit easily into a nucleus tells us that the cell has to develop a method for storing DNA when it's not in use. Biology students know that the method is to wrap DNA in a coil around a protein called a histone; the size of the histone barrel, of course, must be of the order of the persistence length or too much energy would be needed to bend the DNA around it. You may want to check the radius of this biological barrel in a cell biology text.

Some things to think about

1. It's easy to construct your own random walk in one dimension by flipping a coin - "heads" on a flip says take a step to the right along the *x*-axis and "tails" says take a step to the left along the *x*-axis. Literary students may think of *Rosencrantz and Guildenstern are Dead* at this point. Flip a coin repeatedly to sample a few large random walks in one dimension, or forget the coin and just draw out all the configurations explicitly for such a walk with 4 or 5 steps. How fast does the walk approach the ideal limit $\langle r_x^2 \rangle = Nb^2$ for a walk along the *x*-axis?

2. Carrying on with one-dimensional walks, what's the difference between

$\langle \mathbf{r}_x \rangle$	mean value of the end-to-end vector $\mathbf{r}_x$
$\langle \lvert \mathbf{r}_x \rvert \rangle$	mean value of the absolute value of $\mathbf{r}_x$ (*i.e.* its length)
$\langle \mathbf{r}_x^2 \rangle$	mean value of $\mathbf{r}_x \cdot \mathbf{r}_x$,

where $\mathbf{r}_x$ is the end-to-end distance of the walk starting at the origin. Perhaps using data from a walk in part 1 (particularly an explicit 4-step walk), evaluate all of these quantities.