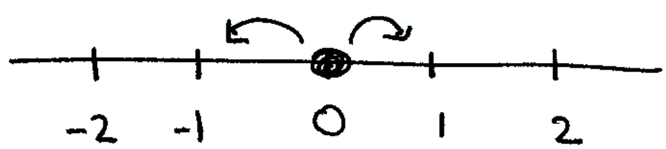
Mar. 30

Random Walks

Most of the discussion in this course will concern system in or close to thermodynamic equilibrium. Very soon, I will have to present to you methods for treating complex systems in equilibrium, and I will need to explain the tricky concept of what 'thermodynamic equilibrium' is. However, it will be good to start our discussion with a simpler problem that involves pure random dynamics. This problem will illustrate how new, simple laws of physics can arise in the large and can be independent of details of microscopic motion.

Consider, then, a *random walk*. The simplest random walk is that on a 1-dimensional lattice. A walker starts at $j = 0$ and takes steps, one after the other, after unit intervals of time. The steps go with equal probability to the left or to the right.



A simple question to ask about this system is: How far from the original position has the walker gone after N steps? I will first give the solution to this problem, and then carry out a more detailed analysis of this process.

At step 0, the walker is certain to be at $j = 0$. At step 1, the walker is at $j = 1$ with probability $\frac{1}{2}$ and at $j = -1$ with probability $\frac{1}{2}$. At step n, we can describe the position of the walker by a probability distribution

$$P_n(j)$$

The total probability that the walker is somewhere is 1, so

$$\sum_{j=-\infty}^{\infty} P_n(j) = 1$$

Also, $P_n(j) = 0$ for $|j| > n$, but, as we will see, this statement is almost irrelevant for large n.

The average position of the walker is

$$\langle j \rangle_n = \sum_j j \, P_n(j)$$

This is obviously equal to zero by symmetry. A more meaningful quantity is the *root mean square deviation* from $j = 0$,

$$\sigma_n \quad \text{such that} \quad \sigma_n^2 = \langle j^2 \rangle_n = \sum_j j^2 \, P_n(j)$$

I hope that, if you are a graduate student in physics, you will immediately guess

$$\sigma_n = \sqrt{n}$$

Here is a proof: Let s_i be random variables that take the values

$$s_i = \begin{cases} +1 & \text{probability } \frac{1}{2} \\ -1 & \text{probability } \frac{1}{2} \end{cases}$$

Then

$$\langle s_i \rangle = 0 \qquad\qquad \langle s_i^2 \rangle = 1$$

We can represent the final position of the walker after n steps as

$$j = \sum_{i=1}^{n} s_i$$

Then

$$\langle j \rangle = \sum_{1}^{n} \langle s_i \rangle = 0$$

$$\langle j^2 \rangle = \sum_{l=1}^{n} s_l \sum_{m=1}^{n} s_m$$

$$= \sum_{l \neq m} s_l s_m + \sum_{l=1}^{n} s_l^2$$

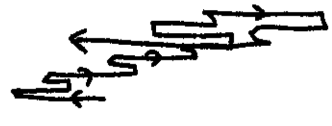
The first term in the last line averages to zero

$$l \neq m \qquad \langle s_l s_m \rangle = \langle s_l \rangle \langle s_m \rangle = 0$$

The second term is equal to n. Thus,

$$\langle j^2 \rangle = n \qquad \sigma_n = \sqrt{n}$$

This means that a typical walk is jagged and backtracking,



Only a rare walk reaches values of j of order n. In fact, the probability that the walker reaches $j = n$ in n steps is exponentially small,

$$P_n(n) = \left(\frac{1}{2}\right)^n = \exp\left[-n \log 2\right]$$

This is the same as the probability that a run of n coin flips turns up all heads.

Here is a somewhat more sophisticated way to obtain the above results. Let

$$K(j, \ell)$$

be the probability that, if the walker started at site ℓ, he ends up at site j after 1 step. It is not hard to write the explicit form of $K(j, \ell)$,

$$K(j, \ell) = \frac{1}{2}\left(\delta_{j,\ell+1} + \delta_{j,\ell-1}\right)$$

If $P_{n-1}(j)$ is the probability distribution of the position of the walker after $(n-1)$ steps, then the position after n steps has the probability distribution

$$P_n(j) = \sum_{\ell} K(j, \ell) P_{n-1}(\ell)$$

This gives a *recursion formula* for $P_n(j)$,

$$P_n(j) = \frac{1}{2}\left[P_{n-1}(j-1) + P_{n-1}(j+1)\right]$$

I will now give three analyses of this recursion formula.

First, we can use the recursion formula to directly compute $\langle j^2 \rangle$.

$$\langle j^2 \rangle_n = \sum_j j^2 P_n(j) = \sum_j \tfrac{1}{2} j^2 \left[P_{n-1}(j-1) + P_{n-1}(j+1) \right]$$

After a change of variables

$$= \sum_j \tfrac{1}{2}\left[(j+1)^2 + (j-1)^2\right] P_{n-1}(j)$$

$$= \sum_j (j^2+1)\, P_{n-1}(j)$$

Thus,

$$\langle j^2 \rangle_n = \langle j^2 \rangle_{n-1} + 1$$

Since $\langle j^2 \rangle_0 = 0$, the recursion gives in a simple way

$$\langle j^2 \rangle_n = n$$

Second, we can use the recursion to solve explicitly for $P_n(j)$. The first few stages are

$P_n(j)$	$j=$ -3	-2	-1	0	1	2	3	..
$n=0$				1				
1			$1/2$		$1/2$			
2		$1/4$		$2/4$		$1/4$		
3	$1/8$		$3/8$		$3/8$		$1/8$	

You can see the pattern building up. The probability $P_n(j)$ is nonzero only when j is *even* for n even, and only when j is *odd* for n odd. And, $P_n(j) = 0$ for $|j| > n$. When $P_n(j)$ is nonzero, its value is

$$P_n(j) = \frac{1}{2^n}\binom{n}{\frac{n+j}{2}} = \frac{1}{2^n}\frac{n!}{\left(\frac{n+j}{2}\right)!\left(\frac{n-j}{2}\right)!}$$

So far, this is a guess, but we can prove it by induction. For $n = 0$, the above formula gives

$$P_0(j) = 1 \quad \text{for } j = 0, \quad 0 \text{ otherwise}$$

as required. Then we are done if we can prove the induction step: If the formula applies to $P_{n-1}(j)$, we must prove that it applies to $P_n(j)$. We can show this by direct calculation:

$$\frac{1}{2}[P_{n-1}(j-1) + P_{n-1}(j+1)] = \frac{1}{2}\frac{1}{2^{n-1}}\left[\frac{(n-1)!}{\left(\frac{n-1+j-1}{2}\right)!\left(\frac{n-1-(j-1)}{2}\right)!} + \frac{(n-1)!}{\left(\frac{n-1+j+1}{2}\right)!\left(\frac{n-1-(j+1)}{2}\right)!}\right]$$

$$= \frac{(n-1)!}{2^n}\left[\frac{1}{\left(\frac{n+j}{2}-1\right)!\left(\frac{n-j}{2}\right)!} + \frac{1}{\left(\frac{n+j}{2}\right)!\left(\frac{n-j}{2}-1\right)!}\right]$$

$$= \frac{(n-1)!}{2^n}\frac{\frac{n+j}{2} + \frac{n-j}{2}}{\frac{n+j}{2}!\left(\frac{n-j}{2}\right)!} = \frac{1}{2^n}\frac{n!}{\left(\frac{n+j}{2}\right)!\left(\frac{n-j}{2}\right)!}$$

and the final step is the required formula; it works!

Using the explicit formula for $P_n(j)$, we can obtain a much clearer picture of the behavior of $P_n(j)$ for large n, j. For large m, the quantity $m!$ can be approximated by *Stirling's formula*

$$m! = m^{m+\frac{1}{2}}\, e^{-m}\sqrt{2\pi}$$

or

$$\log(m!) = (m+\tfrac{1}{2})\log m - m + \tfrac{1}{2}\log 2\pi + O\left(\tfrac{1}{m}\right)$$

(The proof of this formula will appear in the homework.) Applying this formula to our explicit expression for $P_n(j)$, we find

$$\begin{aligned}
\log P_n(j) &= -n\log 2 + \log n! - \log\left(\tfrac{n+j}{2}\right)! - \log\left(\tfrac{n-j}{2}\right)! \\
&= -n\log 2 + (n+\tfrac{1}{2})\log n - n - \left(\tfrac{n+j}{2}+\tfrac{1}{2}\right)\log\tfrac{n+j}{2} \\
&\qquad - \left(\tfrac{n-j}{2}+\tfrac{1}{2}\right)\log\tfrac{n-j}{2} + \tfrac{n+j}{2} + \tfrac{n-j}{2} - \tfrac{1}{2}\log 2\pi + \cdots
\end{aligned}$$

From our earlier estimates, we saw that j is typically of size $\sqrt{n}$ and therefore is typically much less than n. It thus makes sense to approximate the above expression for $|j| \ll n$. Then, for example,

$$\begin{aligned}
\log\tfrac{n+j}{2} &= \log\tfrac{n}{2}\left(1+\tfrac{j}{n}\right) = \log\tfrac{n}{2} + \log\left(1+\tfrac{j}{n}\right) \\
&= \log n/2 + j/n - \frac{j^2}{2n^2} + \cdots
\end{aligned}$$

Using this approximation,

$$\begin{aligned}
\log P_n(j) &= n\log n/2 + \tfrac{1}{2}\log n \text{ [redacted] } \left(\tfrac{n+j}{2} + \tfrac{n-j}{2}\right)\log\tfrac{n}{2} - \tfrac{3}{2}\log n/2 \\
&\qquad - \left(\tfrac{n+j}{2}\right)\left(\tfrac{j}{n} - \tfrac{j^2}{2n^2}\right) - \left(\tfrac{n-j}{2}\right)\left(-\tfrac{j}{n} - \tfrac{j^2}{2n^2}\right) \\
&\qquad - n + \tfrac{n+j}{2} + \tfrac{n-j}{2} - \tfrac{1}{2}\log 2\pi + \cdots
\end{aligned}$$

which now simplifies dramatically

$$\begin{aligned}
&= -\tfrac{1}{2}\log n + \log 2 - \tfrac{1}{2}\log 2\pi \\
&\qquad - \left(\frac{j^2}{2n} - \frac{j^2}{4n}\right)\cdot 2 + \cdots
\end{aligned}$$

and, finally, to

$$\log P_n(j) = -\frac{j^2}{2n} + \log \frac{2}{\sqrt{2\pi n}}$$

or

$$P_n(j) = \frac{2}{\sqrt{2\pi n}} e^{-j^2/2n}$$

One more step is necessary. For n even, the formula we have been analyzing applies only for j even. For j odd, the probability is zero. For n odd, the formula applies only for j odd. But now we are treating j as a continuous variable. It makes sense to define the probability $P_n(j)$ in such a way that

$$[\text{Prob of } j_1 < j < j_2] = \int_{j_1}^{j_2} dj \, P_n(j)$$

For this to be correct, we must average over the even and odd sites. This is a sort of *coarse graining*, ignoring microscopic details to obtain a correct macroscopic probability density. Then the final probability distribution is

$$P_n(j) = \frac{1}{\sqrt{2\pi n}} e^{-j^2/2n}$$

The final probability $P_n(j)$ is a Gaussian distribution. We will be encountering many Gaussian distributions in this course, so it will be good to familiarize yourself with the properties of such distributions. I will write, canonically,

$$g(x) = e^{-x^2/2\sigma^2}$$

Then the first few moments of the distribution are

$$\int_{-\infty}^{\infty} dx \quad e^{-x^2/2\sigma^2} = \sqrt{2\pi\sigma}$$

$$\int_{-\infty}^{\infty} dx \quad x \, e^{-x^2/2\sigma^2} = 0$$

$$\int_{-\infty}^{\infty} dx \quad x^2 \, e^{-x^2/2\sigma^2} = \sigma^2 \cdot \sqrt{2\pi\sigma^2}$$

The first line is the famous result of Liouville[1] The even moments of the Gaussian distribution can be derived by differentiating the first line with respect to σ^2. The odd moments are obviously equal to zero. A properly normalized Gaussian distribution is then

$$G(x) = \frac{1}{\sqrt{2\pi\sigma}} e^{-x^2/2\sigma^2}$$

with

$$\int_{-\infty}^{\infty} dx \quad G(x) = 1$$

$$\int_{-\infty}^{\infty} dx \, x \, G(x) = 0$$

$$\int_{-\infty}^{\infty} dx \quad x^2 \, G(x) = \sigma^2$$

Using the above properties of the Gaussian distribution, we can check that

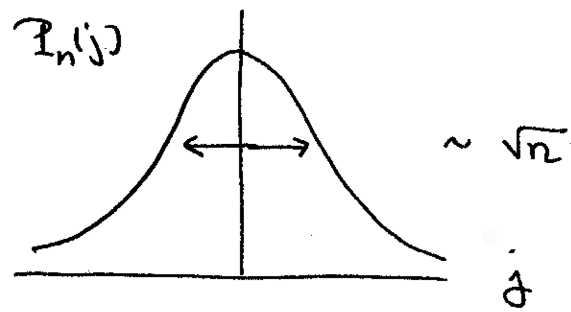
$$\sum_j P_n(j) \cong \int_{-\infty}^{\infty} dj \, \frac{1}{\sqrt{2\pi n}} e^{-j^2/2n} = 1$$

and

[1] Lord Kelvin: "A mathematician is one to whom that is as obvious as that twice two makes four is to you."

$$\langle j^2 \rangle = \sum_j j^2 P_n(j) \cong \int dj \; j^2 \frac{1}{\sqrt{2\pi n}} e^{-j^2/2n} = n$$

But now we can also graph the overall form of $P_n(j)$.



The approximation confirms that $P_n(j)$ gets *very small*, even exponentially small, when $j \sim n$.

I promised you a third way to analyze the recursion formula. To derive it, go back to the equation

$$P_n(j) = \sum_{\ell} K(j,\ell)\, P_{n-1}(\ell)$$

Formally, we can imagine $P_n(j)$ as a vector indexed by j. Then this formula has the form of a matrix K multiplied into this vector. Then we can run the recursion by repeated matrix multiplication. This gives the formal result

$$P_n = [K]^n P_{n=0}$$

The matrix $K(j,\ell)$ depends only on the difference $(j-\ell)$. Thus, we can solve the equation explicitly by Fourier transforming. It is simplest to now go to continuous variables, rewriting the above equations as

$$K(j,\ell) = \frac{1}{2}\left[\delta(j-\ell-1) + \delta(j-\ell+1)\right]$$

and

$$P_n(j) = \int d\ell \; K(j,\ell)\, P_{n-1}(\ell)$$

with

$$P_{n=0}(j) = \delta(j)$$

Now introduce Fourier transforms

$$P_n(j) = \int \frac{dk}{2\pi}\, e^{ikj}\, \tilde{P}_n(k)$$

$$K(j-\ell) = \int \frac{dk}{2\pi}\, e^{ik(j-\ell)}\, \tilde{K}(k)$$

These formulae are inverted by

$$\tilde{P}_n(k) = \int dj\, e^{-ikj}\, P_n(j)$$

$$\tilde{K}(k) = \int dj\, e^{-ikj}\, K(j,0)$$

(I will use these conventions throughout the course in writing Fourier transforms.)

Now plug the Fourier representations into the recursion formula. We find

$$\int \frac{dk}{2\pi}\, e^{ikj}\, \tilde{P}_n(k) = \int d\ell \int \frac{dk}{2\pi}\frac{dk'}{2\pi}\; e^{ik(j-\ell)}\, e^{ik'\ell}\; \tilde{K}(k)\, \tilde{P}_{n-1}(k')$$

Since

$$\int dl \; e^{-ikl} \, e^{ik'l} = 2\pi \, \delta(k-k')$$

the right-hand side of the equation collapses and we find the simple form

$$\tilde{P}_n(k) = \tilde{K}(k) \, \tilde{P}_{n-1}(k)$$

The solution of the recursion formula then takes the form

$$\hat{P}_n(k) = [\tilde{K}(k)]^n \, \tilde{P}_0(k)$$

The initial condition is written in Fourier space as

$$\tilde{P}_0(k) = 1$$

Then

$$\hat{P}_n(k) = (\tilde{K}(k))^n$$

In the problem at hand, the Fourier transform of $K(j, \ell)$ is

$$\tilde{K}(k) = \frac{1}{2}\left(e^{ik} + e^{-ik}\right) = \cos k$$

so

$$\tilde{P}_n(k) = (\cos k)^n$$

Note that

$$\int_{-\infty}^{\infty} dj \; P_n(j) = \tilde{P}_n(k=0)$$

so, quite explicitly,

$$\int_{-\infty}^{\infty} dj \, P_n(j) = 1$$

for all n, as required.

We could go ahead and blindly invert the Fourier transform to find $P_n(j)$. However, the final expression will be clearer if we make some judicious approximations based on the typical size of k. Remember that, for large n, $j \sim \sqrt{n}$, so the Fourier transform variable k will be of order

$$k \sim \frac{2\pi}{\sqrt{n}} \ll 1$$

I propose that we expand

$$\cos k = 1 - \frac{k^2}{2} + \frac{k^4}{4!} + \cdots$$

Then

$$(\cos k)^n = \left(1 - \frac{k^2}{2} + \frac{k^4}{4!} + \cdots\right)^n$$

Or, rescaling to a quantity κ that should remain of order 1,

$$\kappa^2 = n k^2$$

we have

$$(\cos k)^n = \left(1 - \frac{\kappa^2}{2n} + \frac{\kappa^4}{4!\, n^2} + \cdots\right)^n$$

Now use

$$\lim_{n \to \infty} \left(1 - \frac{x}{n}\right)^n = e^{-x}$$

Notice that the κ^n term gives a correction of the order of $1/n$ as $n \to \infty$. If we drop this small correction, we find

$$\tilde{P}_n(k) = e^{-\kappa^2/2} = e^{-\frac{n}{2}k^2}$$

The Fourier inversion of this formula is

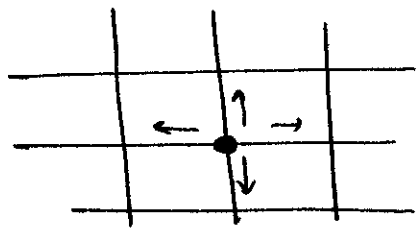
$$P_n(j) = \int \frac{dk}{2\pi}\, e^{ikj}\, e^{-\frac{n}{2}k^2} = \int \frac{dk}{2\pi}\, e^{-\frac{n}{2}\left(k - i\frac{j}{\sqrt{n}}\right)^2}\, e^{-j^2/2n}$$

or, finally,

$$P_n(j) = \frac{1}{\sqrt{2\pi n}} e^{-j^2/2n}$$

the same result as above. Here the approximation for small k or $\kappa \sim 1$ was the coarse-graining step that removed the fine structure present at $k \sim \pi$.

This last argument is very powerful and generalizes to many other random walk problems. Consider, for example, a random walk on a 2-dimensional lattice.



For this problem, the kernel $K(\vec{j}, \vec{\ell})$ that describes one step of the random walk has the form

$$K(\vec{j},\vec{\ell}) = \frac{1}{4}\Big[\, \delta^{(2)}(\vec{j}-\vec{\ell}+\hat{x}) + \delta^{(2)}(\vec{j}-\vec{\ell}-\hat{x}) + \delta^{(2)}(\vec{j}-\vec{\ell}+\hat{y}) + \delta^{(2)}(\vec{j}-\vec{\ell}-\hat{y}) \Big]$$

The 2-dimensional Fourier transform of this quantity is

$$\begin{aligned} \tilde{K}(k) &= \int d^2 j \; e^{-i\vec{k}\cdot\vec{j}} \, K(\vec{j},\vec{0}) \\ &= \frac{1}{4}\left(e^{ik_x} + e^{-ik_x} + e^{ik_y} + e^{-ik_y}\right) \\ &= \frac{1}{2}\left(\cos k_x + \cos k_y\right) \end{aligned}$$

Using this result, we can repeat the argument for a 1-dimensional random walk and find the Fourier transform of the probability distribution as

$$\tilde{P}_n(k) = [\tilde{K}(k)]^n = \left[\frac{\cos k_x + \cos k_y}{2}\right]^n$$

To understand this distribution in the large, we can rescale, defining

$$\kappa_x = \sqrt{n}\, k_x \qquad \kappa_y = \sqrt{n}\, k_y$$

and then concentrate on the region where κ_x, κ_y are of order 1. This approximation to $\tilde{P}_n(\vec{k})$ gives

$$\tilde{P}_n(k) = \left[1 - \frac{\kappa_x^2}{4n} - \frac{\kappa_y^2}{4n} + \frac{\kappa_x^4 + \kappa_y^4}{2 \cdot 4!\, n^2} + \cdots\right]^n$$

$$\longrightarrow \exp\left[-\frac{\kappa_x^2 + \kappa_y^2}{4}\right]$$

with an error of relative order $1/n$. Inverting the Fourier transform, we find

$$P_n(j) = \frac{1}{\pi n}\, e^{-(\vec{j})^2/n}$$

For this distribution

$$\langle j_x^2 \rangle = \tfrac{1}{2} n \qquad \langle j_y^2 \rangle = \tfrac{1}{2} n \qquad \langle (\vec{j})^2 \rangle = n$$

so the distance covered by the random walk still scales like $\sqrt{n}$.

An amazing thing happened in this derivation! Our original problem was not rotational invariant. Its geometry was closely tied to that of the 2-dimensional lattice.

But, when we run the random walk for many steps and loop at the large-scale behavior, we find that the probability distribution is rotationally invariant. We might call this *emergent symmetry.* The symmetry-breaking terms $(k_x^4 + k_y^4)$ are said to be *irrelevant* in considering the large-distance behavior.

In fact, there is an even stronger conclusion that we can draw. Consider *any* random walk for which the Fourier transform of the kernel has a Taylor expansion

$$\tilde{K}(k) = 1 - \tfrac{1}{2}a^2(k_x^2 + k_y^2 + \cdots) + \begin{pmatrix}\text{any behavior} \\ \text{at } \mathcal{O}(k^4)\end{pmatrix} + \cdots$$

According to the argument above, we find that, for all such walks,

$$\tilde{P}_n(k) = e^{-\frac{a^2}{2}k^2\left(1 + \mathcal{O}(\frac{1}{n})\right)}$$

for large n. In d dimensions, the inversion of this Fourier transform gives the following form for the probability distribution,

$$P_n(\vec{j}) = \frac{1}{(2\pi a n)^{d/2}} e^{-|\vec{j}|^2/2na^2}$$

This formula depends on one scale parameter a, which can be identified as the mean square length of a single step,

$$\langle (j_x)^2 \rangle = a^2 \quad \text{in 1 step.}$$

Again, for *any* random walk satisfying this condition, we obtain *the same* large-scale behavior, including rotational symmetry. This phenomenon is called *universality.*

Emergence and *universality* are also properties of systems of many interacting particles or degrees of freedom as viewed in the large. We will meet these concepts again in our study of statistical mechanics.