Physics 112 : Lecture 2

Notes for the Fall 2017 Physics 112 Course taught by Professor Holzapfel
prepared by Joshua Lin (email: joshua.z.lin@gmail.com)

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1 One Dimensional Random Walks

Though they are simple, random walks are very useful models in thermodynamics that helps us model many different situations. For example, we might be interested in diffusion (the phenomenon where particles which are at first locally concentrated spread out due to thermal motion), or brownian motion[1] (where we investigate the paths of single particles that are continuously bombarded on all sides by particles in their environment; e.g. a grain of pollen in a glass of water). An example we will cover today will be a collection of spin-half particles (such as the particles that constitute a para-magnetic substance), where each particle is either spin up or spin down; but the total magnetism of the substance is determined by the net amount of spin up particles minus the net amount of spin down particles.

For now, let us consider a One Dimensional Random Walk. We model this by letting a particle start at $x = 0$, and at every step the particle has p chance that the particle goes to the right by one unit, and q chance that the particle goes to the left by one unit. We will assume that $p + q = 1$, i.e. that at every step the particle either goes left or right, and cannot stay still. After N steps, one possible outcome could be:

$$LLRRLRLRRR...LLR$$

where L represents the particle going to the left on that step, and R represents the particle going to the right on that step. If we wanted to find out the probability that this particular path was taken by the particle, we'd need to multiply all the probabilities together:

$$P = qqppqpqppp...qqp$$

We call each particular path a 'microstate' of the system. We can represent the probability above in a more compact manner, suppose we let n_1 be the number of times the particle steps to the right, and n_2 be the number of times that the particle steps to the left. Evidently $n_1 + n_2 = N$, since there were N steps in total. So we can write:

$$P = p^{n_1} q^{n_2}$$

[1]Mathematically, 'random walks' usually describe discrete processes, but when we model things like Brownian Motion we often need to use continuous models; usually through stochastic calculus and measure theory

What if we are in the situation where we don't actually care *how* the particle gets to its endpoint (i.e. we don't care which particular path the particle takes, we don't care about the specific microstate), but we only care about where the endpoint actually is? Specific endpoints of the particle are called 'macrostates', and are the things that are usually much easier to observe from a system. As a first question, we might ask how many microstates correspond to a specific macrostate for our one dimensional random walk? We can label our macrostates by m (i.e. the macrostate m corresponds to the particle ending at $x = m$ after N steps). First notice that:

$$m = n_1 - n_2; \qquad n_1 = \frac{1}{2}(N+m); \qquad n_2 = \frac{1}{2}(N-m)$$

So the number of different microstates corresponding to the macrostate m is given by:

$${}^{N}C_{n_1} = {}^{N}C_{\frac{1}{2}(N+m)}$$

since out of the N different steps we want n_1 of them to be to the right[2], where n_1 is given by the formula derived earlier. Now, we can find the probability of a specific macrostate occurring:

$$P_N(m) = {}^{N}C_{n_1} p^{n_1} q^{n_2} = {}^{N}C_{\frac{1}{2}(N+m)} p^{\frac{1}{2}(N+m)} q^{\frac{1}{2}(N-m)}$$

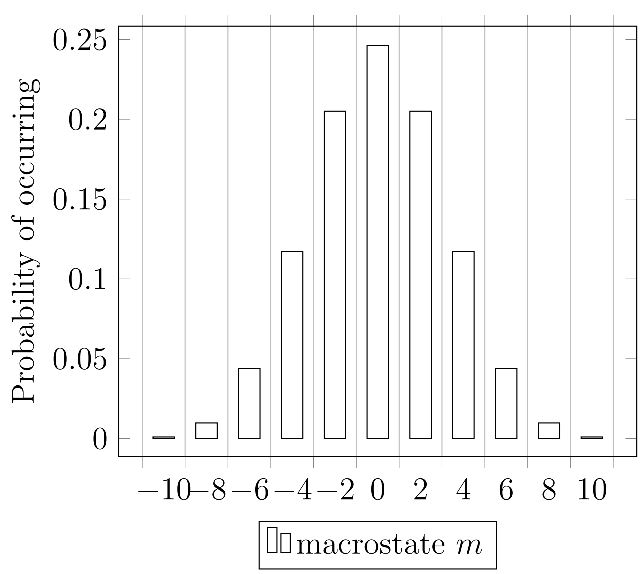
where we multiply the number of microstates corresponding to the macrostate by the probability of each microstate of occurring.

There is also an alternate way of understanding one dimensional random walks. Consider the binomial expansion:

$$(p+q)^N = \sum_{n=0}^{N} {}^{N}C_n p^n q^{N-n}$$

Note that each term in the sum on the right hand side of the equation looks exactly like the probability of the macrostate $m = 2n_1 - N$ occuring in our one dimensional random walk.

Below, we have the diagram for the case where $N = 10$, the different probabilities of being in each macrostate. Note that already it is peaked near $m = 0$.



[2]Note that we could have also chosen n_2 of the steps to be to the left, since ${}^{N}C_{n_1} = {}^{N}C_{N-n_1} = {}^{N}C_{n_2}$

2 Magnetism

We can apply our one dimensional random walk model to the problem of magnetism (at least in the paramagnetic case; for systems like ferromagnetism where all the particles interact with each other then it gets more complicated). Here, instead of having a particle take N steps on a one dimensional line, we have N different particles, each of which can be spin up or spin down. If a particle is spin up, then it has magnetic moment $+m$, and if it is spin down, then it has magnetic moment $-m$. [3] Now, the total magnetic moment of the N particles is given by:

$$M = (N_\uparrow - N_\downarrow)m$$

where $N_\uparrow$ is the number of particles that are spin up, and $N_\downarrow$ is the number of particles that are spin down. It's clear then that:

$$-Nm \leq M \leq Nm$$

and that there are $N+1$ different values that M can take. In this situation, to make the notation cleaner we don't actually use different values of M as our macrostates, but rather we define:

$$2s = N_\uparrow - N_\downarrow$$

as the 'spin excess', and use different values of s as our macrostates. At this stage, we can apply all that we learnt previously about one dimensional random walks to this new system. Now, we define $g(N,s)$ to be the multiplicity of the macrostate s with N particles, i.e. how many different microstates of N particles correspond to the macrostate s. It's clear that:

$$g(N,s) = {}^N C_{N_\uparrow} = \frac{N!}{N_\downarrow! N_\uparrow!}$$

but for large N (larger than the order of 10^{20} or so), this number becomes so large and intractable to compute, that we consider the logarithm of $g(N,s)$ instead, so that we may apply some nice approximations.

3 Mathematical Approximations

From the properties of logarithms, we know that:

$$\ln(ab) = \ln(a) + \ln(b); \qquad \ln\left(\frac{a}{b}\right) = \ln(a) - \ln(b)$$

Hence to find the logarithm of our system, we have:

$$\ln(g(N,s)) = \ln\left(\frac{N!}{(N/2+s)!(N/2-s)!}\right) = \ln[N!] - \ln[(N/2+s)!] - \ln[(N/2-s)!]$$

[3] Note that this m represents a physical constant, the magnetic moment of a particle, and is not in any way related to our other m from earlier, which represented the macrostate of our one dimensional walk

For large N, Stirling's approximation (which wasn't proved in lecture) tells us that:

$$N! \approx (2\pi N)^{\frac{1}{2}} N^N \exp[-N + \frac{1}{12N} + \cdots]$$

So applying the logarithm we have:

$$\ln(N!) \approx \frac{1}{2}\ln(2\pi) + \left(N + \frac{1}{2}\right)\ln N - N$$

If we apply this approximation to our expression for $\ln(g(N,s))$, we find that:

$$\begin{aligned}
\ln(g(N,s)) &= \frac{1}{2}\ln(2\pi) + \left(N + \frac{1}{2}\right)\ln N - N \\
&- \left[\frac{1}{2}\ln(2\pi) + \left(\frac{N}{2} + s + \frac{1}{2}\right)\ln(N/2+s) - (N/2+s)\right] \\
&- \left[\frac{1}{2}\ln(2\pi) + \left(\frac{N}{2} - s + \frac{1}{2}\right)\ln(N/2-s) - (N/2-s)\right] \\
&= -\frac{1}{2}\ln(2\pi) + (N+1/2)\ln N \\
&- (N/2+s+1/2)\left[\ln N + \ln(1+2s/N) - \ln 2\right] \\
&- (N/2-s+1/2)\left[\ln N + \ln(1-2s/N) - \ln 2\right] \\
&= \frac{1}{2}\ln(2\pi) - \frac{1}{2}\ln N + (N+1)\ln 2 - \left(\frac{2s}{N}\right)^2
\end{aligned}$$

where we use the logarithm laws discussed earlier, and in the last step we exploit the expansion

$$\ln(1+x) \approx x - \frac{1}{2}x^2 + \cdots$$

for small x. (so we are assuming here that s is much less than N). If we exponentiate this expression again, we recover an approximation for our multiplicity function:

$$g(N,s) \approx \left(\frac{2}{\pi N}\right)^{1/2} 2^N e^{-(2s/N)^2}$$

Note that this function looks like a gaussian in s, so it drops off relatively fast as s deviates from zero.

For a fun one dimensional random walk problem; suppose we formalize a random walk as $\sum_{i=1}^N X_i$ where each X_i is an independent identical random variable, which is $+1$ with probability p and -1 otherwise. Find the average size of the set $\{\sum_{i=1}^j X_i | 1 \leq j \leq N\}$ as a function of N, i.e. the average size of the set of positions that the particle visits in N steps.