Lectures on the random walk

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Opening statment: generalities

I have been told that I can talk about whatever I want, as long as it has to do with random walks. This is fine with me. However, it leaves me with a bit of a dilemma. There is so much to say about the subject and three lectures does not give me all that much time. I think that what I will do is focus on a few topics that amuse me and that I think you will find interesting and useful as well. My first job will be to provide a general introduction to the subject and in particular to convince you of the importance and utility of a few key concepts and approaches, principle among them the method of the **generating function**. For those of you who are interested in pursuing the subject further, there are a number of excellent books. However, given that I like many others operate from a position of healthy self-interest, let me refer you to a book co-authored by me on the subject [Rudnick and Gaspari, 2004].

We will start with the discussion of some basic quantities.

The random walker

First, we need to talk about what the random walker is, exactly. The simplest version of a random walker is that that it is something that takes a set of successive steps and that the direction in which it moves is, to some extent, random. In the simplest, "ideal," case, the direction is *entirely* random. This leaves open two other questions

1. How much ground does the walker cover at each step? Is this quantity fixed or random?

2. Does the walker take the steps in a regular time sequence (e.g. a step each and every second) or is there randomness in that choice as well?

Again, in the simplest case the length of each step is fixed and the walker takes steps at regular time intervals. We will consider variations on the above standard set of conditions later on.

Number of walks

Now we turn to quantities of fundamental interest in discussions of the properties of random walkers and random walks. The most widely used, and generally most widely applicable, of those quantities is the number of random walk, assuming that certain conditions apply. For example, consider the following simple question:

> A random walker starts at the location $\vec{x}$, takes N steps and ends up at the location $\vec{y}$. How many ways are there for this to happen?

A bit more concisely and technically: how many N-step walks are there that start at $\vec{x}$ and end at $\vec{y}$? Figure 1 shows three random walks starting and ending at the same point. The question is, how many of such paths are there? This quantity, which we'll call $C(N; \vec{x}, \vec{y})$ plays the same role in random walk

Figure 1: Three random walks starting and ending at the same point.

statistics as the partition function plays in statistical mechanics. To see what

I mean by this, consider the following definition of the partition function

$$\mathcal{Z}_N = \sum_{N-\text{particle states}} e^{-\beta E_{\text{state}}} \tag{1}$$

where the sum above is–as clearly indicated–over all of the states of a given N-particle system. The exponential is the standard Boltzmann factor, β being $1/k_B T$ and E_{state} the energy of the given state. By comparison, the quantity $C(N; \vec{x}, \vec{y})$ is given by the equation

$$C(N; \vec{x}, \vec{y}) = \sum_{N-\text{step walks starting at } \vec{x} \text{ and ending at } \vec{y}} \tag{2}$$

In the case of the sum on the right hand side of (2), the "Boltzmann factor" is one. We can alter this if the conditions on the walk change, and in fact we will do so shortly.

Recursion relations

So, how do we evaluate the sum in question? One very useful method makes use of a relationship between the number of N step walks and the number of walks that require $N+1$ steps. The argument leading to this relationship is fairly transparent. Here is how it goes. If I have managed to find out how many N-step walks start at a given point $\vec{x}$ and terminate at all possible end points $\vec{y}'$, then counting all $N+1$ step walks starting at $\vec{x}$ and terminating at a particular end point $\vec{y}$ just involves adding up all N step walks that start at $\vec{x}$ and end up at a point from which the walker can get to y in one step. Suppose I know the value of $C(N; \vec{x}, \vec{y})$ for all endpoints, $\vec{y}$. Then, $C(N+1, \vec{x}, \vec{y})$ equal is given by

$$C(N+1; \vec{x}, \vec{y}) = \sum_{\vec{w}_i} C(N; \vec{x}, \vec{w}_i) \tag{3}$$

Here, the $\vec{w}_i$'s are the locations of the points from which the walker can make it to the location $\vec{y}$ in one step. Figure 2 illustrates of the process summarized in Eq. (3)[1].

[1] In the figure, as noted in the caption, the process depicted is appropriate to a random walker on a lattice. In general, I will not be precise about whether this assumption applies, as most results are qualitatively independent of that particular restriction

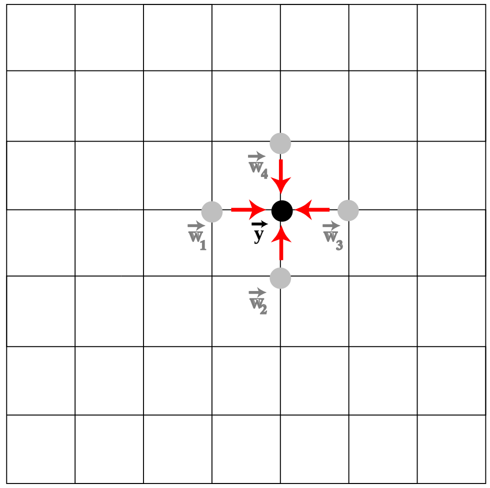

Figure 2: An illustration of the recursion relation summarized in Eq. (3). Here, the random walker is confined to the vertices of a two-dimensional lattice and all steps are between a lattice point and its nearest neighbor.

If we play some games with this recursion relation, we end up with a useful, general and nearly ubiquitous equation. The key assumption is going to be that we can make use of power series expansions. First, we'll assume that we can express the dependence of the number of walks on the number of steps taken in terms of a Taylor expansion in the latter quantity. This means we can write

$$C(N+1;\vec{x},\vec{y}) = C(N;\vec{x},\vec{y}) + \partial C(N;\vec{x},\vec{y})/\partial N + \cdots \tag{4}$$

Furthermore, we will assume that the same sort of expansion is possible with respect to the locations of the starting and ending points. Let's focus our attention on the kind of walk on a lattice shown in Fig. 2. Given that we can write

$$\begin{aligned} \vec{w}_i &= \vec{y} + (\vec{w}_i - \vec{y}) \\ &\equiv \vec{y} + \vec{\Delta}_i \end{aligned} \tag{5}$$

we can then replace the right hand side of the recursion relation equation (3) by

$$
\begin{aligned}
&\sum_{\Delta_i} C(N;\vec{x},\vec{y}+\vec{\Delta}_i) \\
&= \sum_{\vec{\Delta}_i} \left(C(N;\vec{x},\vec{y}) + \vec{\Delta}_i \cdot \vec{\nabla}_y C(N;\vec{x},\vec{y}) + \frac{1}{2}\sum_{l,m} \Delta_{i,l}\Delta_{i,m}\frac{\partial^2}{\partial y_l \partial y_m} C(N;\vec{x},\vec{y}) + \cdots \right)
\end{aligned} \tag{6}
$$

where $\Delta_{i.m}$ is the m^{th} component of the vector displacement $\vec{\Delta}_i$. To continue in our analysis of the random walk along these lines, we will consider the case of a walker restricted to the vertices of a cubic lattice. This means that the $\vec{\Delta}$'s are aligned the the x, y or z axis. Because of this, we have the following results

$$\sum_{\vec{\Delta}_i} = 6 \tag{7}$$

$$\sum_{\vec{\Delta}_i} = 0 \tag{8}$$

$$
\begin{aligned}
\sum_{\vec{\Delta}_i}\sum_{l,m} \Delta_{i,l}\Delta_{i,m}\frac{\partial^2}{\partial y_l \partial y_m} &= 2a^2 \left(\frac{\partial^2}{\partial y_1^2} + \frac{\partial^2}{\partial y_2^2} + \frac{\partial^2}{\partial y_3^2} \right) \\
&= a^2 \vec{\nabla}_y^2
\end{aligned} \tag{9}
$$

The quantity a on the right hand side of (9) is the magnitude of each $\vec{\Delta}_i$, and y_k is the k^{th} component of the position vector $\vec{y}$.

Collecting all the results together, we are left with the following equation for the quantity $C(N;\vec{x},\vec{y})$.

$$
\begin{aligned}
&C(N;\vec{x},\vec{y}) + \partial C(N;\vec{x},\vec{y})/\partial N \\
&= 6C(N;\vec{x},\vec{y}) + a^2 \vec{\nabla}_y^2 C(N;\vec{x},\vec{y})
\end{aligned} \tag{10}
$$

Rearranging, we end up with the following partial differential equation

$$\frac{\partial C(N;\vec{x},\vec{y})}{\partial N} = 5C(N;\vec{x},\vec{y}) + a^2 \nabla_y^2 C(N;\vec{x},\vec{y}) \tag{11}$$

This looks a lot like the Schrödinger equation for a particle in a constant potential. The principal difference is that the number of steps, N, plays the role of an *imaginary* time. As it turns out, the equation is not quite right. We have made too much of an approximation in utilizing the first two terms in the Taylor expansion in N in our treatment of the left hand side of the recursion relation. To see this, let's figure out what the equation tells us about the number of N-step walks that start at x and end up anywhere. We do this by simply summing over end-points, y. Making use of the fact that the last term on the right hand side of (11) can be expressed in terms of perfect derivatives,and that the integral over all $\vec{y}$ of the function $C(N;\vec{x},\vec{y})$ converges, because when $\vec{y}$ is sufficiently far from $\vec{x}$ no N-step walk will connect the two points, we have on integrating both sides of (11) over $\vec{y}$

$$\frac{\partial}{\partial N}\int C(N;\vec{x},\vec{y})d^3y = 5\int C(N;\vec{x},\vec{y})dy \tag{12}$$

or, defining

$$\mathcal{C}(N;\vec{x}) = \int C(N;\vec{x},\vec{y})dy \tag{13}$$

$$\frac{\partial\mathcal{C}(N;\vec{x})}{\partial N} = 5\mathcal{C}(N;\vec{x}) \tag{14}$$

The solution to this equation is

$$\mathcal{C}(N;\vec{x}) = \mathcal{C}(0;\vec{x})e^{5N} \tag{15}$$

Equation (15) tells us that the number of N step walks increases exponentially in the number of steps. Does this make sense? Consider the process. At each step, the walker on the cubic lattice has a choice of six neighboring sites to visit. This means that the total number of walks increases by a factor of 6 at each step, or the total number of N step walks goes as $6^N = e^{N\ln 6}$. This is qualitatively consistent with the result displayed in (15). Is it quantitatively consistent? According to that result the number of walks increases by the factor $e^5 = 148.4$ at each step. We are right about the exponential growth in the number of walks with steps taken but wildly off with respect to the actual rate of exponential increase. The moral is cautionary. Be careful when you treat a discrete quantity as if it were continuous.

There is another quantity related to the number of N-step walks for which the kind of equation displayed in (11) is absolutely relevant and asymptotically correct. This quantity is equal to the *fraction* of N-step walks starting at $\vec{x}$ and ending at $\vec{y}$. To obtain this quantity, we divide $C(N;\vec{x},\vec{y})$ by the total number of N step walks, which we've seen is 6^N. Let's call this quantity $D(N;\vec{x},\vec{y})$. The recursion relation corresponding to (3) is

$$D(N+1,\vec{x},\vec{y}) = \frac{1}{6}\sum_{\vec{w}_i} D(N;\vec{x},\vec{w}_i) \tag{16}$$

Carrying out the same truncated Taylor expansions as before, we end up with the differential equation

$$\frac{\partial D(N;\vec{x},\vec{y})}{\partial N} = \frac{a^2}{6}\nabla_y^2 D(N;\vec{x},\vec{y}) \tag{17}$$

If we integrate both sides of this equation with respect to $\vec{y}$, we end up with the quite proper result

$$\frac{\partial}{\partial N}\int D(N;\vec{x},\vec{y})d^3y = 0 \tag{18}$$

This tells us that if we sum the fraction of walkers that end up at a given site over all possible end points, we end up with a constant. In fact, we know that the constant in question is one.

Now, (17) is a well known and widely studied equation. It is, in fact the **diffusion equation**. Among other phenomena, it describes the spreading of a cloud of suspended particles in a liquid or vapor host, an example being a drop of ink or dye that has been deposited in water. This allows for another interpretation of the function $D(N;\vec{x},\vec{y})$. Imagine a collection of walkers that have al been simultaneously deposited at the point $\vec{x}$. They then walk, in the simplest case all in lockstep, out from that point. The quantity $D(N;\vec{x},\vec{y})$ is the concentration of those walkers, normalized to one. Figure 3 shows the case when there are only five walkers, after they have taken 100 steps.

This interpretation of the function will help lead us to some very useful approaches to classic problems.

Solution of the diffusion equation

Given our new, and very familiar looking equation, let's solve it. If you have gone through the exercise of calculating the evolution of the wave packet of a free quantum mechanical particle then the steps below will be very familiar. We start by Fourier transforming the equation (17) in space. Explicitly, we conjecture a solution to the equation of the form

$$D(N;\vec{x},\vec{y}) = d(N,\vec{q})e^{i\vec{q}\cdot(\vec{y}-\vec{x})} \tag{19}$$

Figure 3: Five random walkers have stated at a common point and have taken 100 steps away from it.

This leads to the following differential equation for the function $d(N, \vec{q})$

$$\frac{\partial d(N, \vec{q})}{dN} = -\frac{a^2 q^2}{6} d(N, \vec{q}) \tag{20}$$

The solution to this equation is

$$d(N, \vec{q}) = d(0, \vec{q}) e^{-a^2 q^2 N/6} \tag{21}$$

The next step is to reconstitute the full solution by taking a superposition of the $d(N, \vec{q})$'s. We can do this, given knowledge of the form of $D(N; \vec{x}, \vec{y})$ at $N = 0$, i.e. before the first step has been taken. A standard initial condition, in fact one consistent with the scenarios described above, has the $D(0; \vec{x}, \vec{y}) = \delta(\vec{y} - \vec{x})$. Given what we know about the Fourier transform of the Dirac delta function, we then have $d(0, \vec{q}) = (2\pi)^{-3}$ for all $\vec{q}$, and

$$\begin{aligned} D(N; \vec{x}, \vec{y}) &= \int d(0, \vec{q}) e^{i\vec{q}\cdot(\vec{y}-\vec{x}) - a^2 N q^2/6} d^3 q \\ &= \frac{1}{(2\pi)^3} \int e^{i\vec{q}\cdot(\vec{y}-\vec{x}) - a^2 q^2/6} d^3 q \end{aligned}$$

$$= \frac{1}{(2\pi)^3}\left(\frac{6\pi}{a^2N}\right)^{3/2} e^{-3|\vec{y}-\vec{x}|^2/2a^2N} \tag{22}$$

In getting to the last line of (22), I made use of the fact that the integral over $\vec{q}$ can be broken up into three independent integrations of the components of that vector and then of the classic result for Gaussian integrations

$$\int_{-\infty}^{\infty} e^{Ax-Bx^2}dx = \sqrt{\frac{\pi}{B}}e^{A^2/4B} \tag{23}$$

Three properties of the solution are worth noting:

1. It is in the form of a Gaussian.

2. Its width scales with $\sqrt{N}$.

3. Its value at the origin goes as $N^{-3/2}$.

All three properties represent key qualitative features of diffusion and the random walk. As a test of the validity of our expression, we can integrate the expression on the last line of (22) over all values of $\vec{y}$. Making use of (23), we verify that $\int D(N;\vec{x},\vec{y})d^3y = 1$.

Given our solution for $D(N;\vec{x},\vec{y})$, what can we say about the original quantity of interest, $C(N;\vec{x},\vec{y})$? In light of the relationship between the two, it is almost a triviality to obtain the second function from the first. In fact, we have

$$\begin{aligned} C(N;\vec{x},\vec{y}) &= 6^N D(N;\vec{x},\vec{y}) \\ &= \frac{6^N}{(2\pi)^3}\left(\frac{6\pi}{a^2N}\right)^{3/2} e^{-3|\vec{y}-\vec{x}|^2/2a^2N} \end{aligned} \tag{24}$$

This tells us that the number of N step walks starting at $\vec{x}$ and ending at $\vec{y}$ has the first two properties listed above, and additionally increases exponentially in the number of steps. In fact a general feature of random walks will be this exponential growth in the number of possibilities with the number of steps. The power-law modification at the origin that is noted as the third item in the list should also be kept in mind.

The current density of walkers

In the case of dye particles diffusing in water, we can express the invasion of those impurities in terms of a current density, through the continuity equation

$$\frac{\partial d}{\partial N} = -\vec{\nabla} \cdot \vec{j} \tag{25}$$

In light of Eq. (17), we can easily intuit the current density

$$\vec{j} = -\frac{a^2}{6}\vec{\nabla}_y D(N; \vec{x}, \vec{y}) \tag{26}$$

The relationship (26) between current density and the density of diffusers is an example of **Fick's Law**.

Suppose, now that there is an absorber, say a wall that sucks up any walker that hits it. How does that effect the density of walkers? We know that the overall effect has to be to decrease them, as walkers that hit the wall are removed from the distribution. Without going into details, allow me to simply say that the consequence on the density of walkers is to force it to zero at the points of impact of the walkers and the absorber. To be more precise, the density extrapolates to zero just beyond the point of impact, but the difference between the more proper and precise effect and the effective boundary condition that we will apply is not important for the phenomena that will be discussed here.

Let's start by considering the case of a walker, or a collection of walkers, that begin some distance from an absorbing wall. We want a distribution that starts out as a delta function, that obeys the equations above in the region in which the walkers take their steps and that obeys the boundary conditions that were asserted above at the wall. To be specific, let's look at the case of a collection of walkers that start out a distance l from a wall that occupies the plane $x_1 = 0$. The walkers start out in the half space $x > 0$. We will locate the starting point at $(l, 0, 0)$. Then, the solution for the distribution $D(N; \vec{x}, \vec{y})$ that is consistent with the boundary conditions is

$$\begin{aligned} D(N; \vec{x}, \vec{y}) &= \frac{1}{(2\pi)^3}\left(\frac{6\pi}{a^2 N}\right)^{3/2} \\ &\quad \times \left(e^{-3((y_1-l)^2+y_2^2+y_3^2)/2a^2N} - e^{-3((y_1+l)^2+y_2^2+y_3^2)/2a^2N}\right) \end{aligned} \tag{27}$$

This is reminiscent of the image charge solution for the electrostatic potential in the presence of a conducting surface. In fact, one way to derive it is to posit the existence of "image walkers" that meet and annihilate walkers that impinge on the absorbing surface. See Fig. 4

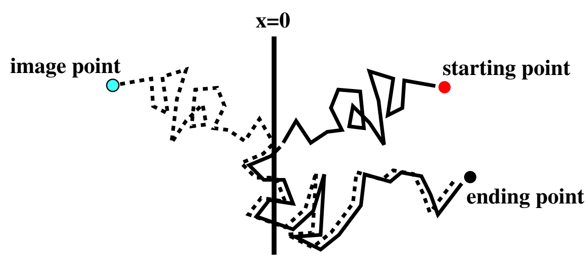

Figure 4: Illustrating the way in which an image walker eliminates a path by the original walker that passes over the boundary at $x = 0$. For every path which crosses the boundary and returns to the ending point, there is a path starting at the image point that can reach the same ending point in the same number of steps, N. This is not the case for walks that do not cross the boundary. Note that the portion of the image walker's path that precedes its first contact with the boundary is the mirror image of the corresponding portion of the real walker's path and that after that first contact the image walker shadows the real one.

Steady state distributions and boundary conditions

We can make even closer contact to the image charge method, and in fact to the calculation of electrostatic potentials, by altering the situation associated with a swarm of walkers. The equation (17) expresses the fact that the only way in which the distribution of walkers will change is through the propagation of walkers into or out of the region in which the distribution is being monitored. Suppose, alternatively, that walkers are steadily being inserted. That is, suppose we amend the equation governing the distribution of walkers by introducing a source term. This leads to a change in both (17) and the equations following from it and to the continuity equation (25). Here is our new version of (17)

$$\frac{\partial D(N;\vec{x})}{\partial N} = \frac{a^2}{6}\nabla^2 D(N;\vec{x}) + s(N,\vec{x}) \tag{28}$$

The last term on the right hand side of (28) is the new source term. Now, let's take the source term to be independent of N, so that walkers are being introduced at a steady rate. Given this, let's see what the distribution of walkers settles down to. That is, let's see what the steady state distribution is, corresponding to a constant infusion of walkers diffusing out from the locations at which they are being introduced. In this case, both s and D are independent of N, and (28) becomes

$$\frac{a^2}{6}\nabla^2 D(\vec{x}) = -s(\vec{x}) \tag{29}$$

Here, I have removed N from the equation, as there is no dependence on that quantity.

Of course, we have all seen Eq. (29). It is Laplace's equation. We all know how to solve it in special cases. If the source term is a delta function, corresponding to the introduction of walkers at a particular point in space, say at $\vec{x} = 0$, then

$$D(\vec{x}) = \frac{3}{2\pi a^2}\frac{1}{|\vec{x}|} \tag{30}$$

The steady state distribution of walkers is governed by the same equation, and it takes on the same form, as the electrostatic potential. Let's make use of this fact to consider a couple of classic problems associated with the random walk.

Gambler's ruin

The problem of the gambler's ruin has been cited by Montroll and Shlesinger as the first example of a situation that can be analyzed in terms of a random walk [Montroll and Shlesinger, 1983]. The solution is due to the celebrated mathematician de Moivre. The question being asked is the following one. Given a game of chance between two players in which neither one has an advantage, suppose the first player starts out with an amount of money equal to A and the second player has an amount of money equal to B. Each will play until he or she has either won all the money or has exhausted his or her resources. What is the likelihood that the first player will walk away the winner?

A way to think of the problem is in terms of a random walker in one dimension that starts off in a bounded interval. The walker is a distance

A from one of the boundaries and B from the other one. As soon as the walker hits one of the boundaries it is absorbed, corresponding to the "ruin" of one of the gamblers. Now, to apply the steady state model to the analysis of Gambler's Ruin, we imagine a constant source of walkers at the starting point, located at $x = A$ as shown in Fig. 5. This replaces the single pair of gamblers by an ensemble of them. We can think of having a very large tournament in which games are being started at a constant rate and continued until a player is out of money. This source leads to a steady state distribution

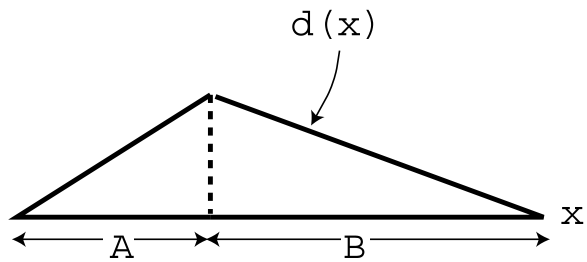

Figure 5: The source, at the location of the vertical dashed line, induces the steady state distribution $d(x)$, as shown.

of walkers, also indicated in the figure. The distribution of walkers, $d(x)$ obeys the one dimensional version of the Poisson equation of electrostatics:

$$\begin{aligned} \frac{a^2}{6}\frac{d^2 d(x)}{dx^2} &= -s(x) \\ &= s_0 \delta(x - A) \end{aligned} \tag{31}$$

Given that the density of walkers vanishes at the absorbing boundaries, we can figure out the solution to this equation. As the second derivative is equal to zero, we know that $d(x)$ has to be a linear function. The delta function generated by the second derivative is the consequence of a discontinuity in the slope of the function. If the function itself were discontinuous at $x = A$, then its first derivative would give rise to a delta function and the second to the derivative of a delta function. This means that $d(x)$ has the form

$$d(x) = \begin{cases} \frac{K}{A}x & 0 < x < A \\ \frac{K}{B}(A + B - x) & B < x < A + B \end{cases} \tag{32}$$

The coefficient K follows from matching the magnitude of the slope discontinuity, $K(1/A + 1/B)$, to the required amplitude of the delta function.

Fortunately for the purposes of completing our analysis we do not need to work out the value of K. We simply need to ratio of random walker currents, and this is easy given (26). According to that version of Fick's law, we have for the walker current density

$$\begin{aligned} j(x) &\propto -\frac{d}{dx}d(x) \\ &\propto \begin{cases} -1/A & 0 < x < A \\ 1/B & A < x < A+B \end{cases} \end{aligned} \tag{33}$$

In other words, walkers are going off the the left and eventually being absorbed by the boundary at $x = 0$ at a relative rate $1/A$, while walkers are wandering off to the right at a relative rate equal to $1/B$. As exit to the left corresponds to the ruin of the gambler with resources amounting to A, while exit to the right corresponds to success for that gambler and ruin for the gambler that starts with an amount equal to B. Let's call the first gambler Gambler A and the second one Gambler B. Then the probability P_A that Gambler A wins divided by the probability that Gambler B wins is given by

$$\begin{aligned} \frac{P_A}{P_B} &= \frac{1/B}{1/A} \\ &= \frac{A}{B} \end{aligned} \tag{34}$$

The gambler with more resources is more likely to win, and the relative likelihood is equal to the ratio of initial resources.

And that is why you are statistically doomed to lose in Las Vegas. Even if the odds are not against you, unless you can match the resources of the house you will eventually end up on the short end.

Walkers near an absorbing sphere

We can also ask what happens to walkers in the vicinity of an absorbing sphere. First, we'll look at the case of a collection of walkers that are supplied by a set of sources that are infinitely far away from the sphere. The sources are such that the distribution of walkers is uniform at an infinite distance from the sphere. To find what the concentration of walkers is at an arbitrary distance from the sphere, which has a radius equal to r_0, we search for a solution of Laplace's equation (because there are no sources in the region of interest) that is equal to zero at the surface of the sphere and that is a constant infinitely far away from the sphere. Placing the origin at the center of the sphere, we can also demand spherical symmetry about that origin. The solution of interest is then readily intuited. It is

$$d(\vec{r}) = c_0 \left(1 - \frac{r_0}{r}\right) \tag{35}$$

where r is the distance from the center of the sphere, and the expression on the right hand side of (35) holds when $r > r_0$.

We can use this formula to calculate the rate at which the walkers are absorbed by the sphere. To do this, we calculate the current density of walkers by taking the gradient of the right hand side of (35), and then by calculating the current flux into the sphere. From (26), we have

$$\begin{aligned} \vec{j}(\vec{r}) &= -\beta\hat{r}\frac{\partial}{\partial r}c_0\left(1 - \frac{r_0}{r}\right) \\ &= -\hat{r}\frac{\beta c_0 r_0}{r^2} \end{aligned} \tag{36}$$

where I have replaced the constant depending on the size of the walker's step by the all-purpose symbol β. This tells us that the flux of walkers into the sphere is equal to

$$\beta c_0 \frac{r_0}{r_0^2} \times 4\pi r_0^2 = 4\pi\beta c_0 r_0 \tag{37}$$

We learn that the number of walkers that are absorbed by the sphere scales linearly with the radius of the sphere. If the sphere represents a cell, and the walkers are nutrients in the broth in which the cell sits, the rate at which the cell takes those nutrients in is proportional to its linear size. On the other hand, if the sphere really is a cell, it has metabolic requirements that scale as its volume—in other words, as r_0^3. Ultimately, those requirements will overwhelm the cell's ability to absorb nutrients through diffusion, as the size of the cell increases. In the case of an immobile cell, these considerations place a limit on the maximum size that it can be. In general, the fact that metabolic needs will exceed the rate at which nutrients can be gathered as they diffuse inwards will mandate a different strategy for the acquisition of biological fuel for any organism that is larger than a certain size [Berg, 1993].

It is also possible to calculate the distribution of walkers when there is a point source outside of an absorbing sphere. In this case, we make use of a modification of the image charge. If the source is a distance R away from the center of a sphere with radius r_0, then the image source is a distance $\rho = r_0^2/R$ from the center of the sphere, and the "strength" of the source is equal to $-r_0/R$ times the strength of the original, external source. It is possible to calculate how many of the walkers escape from the sphere by taking the integral of the current flux through a surface that surrounds both the source and the absorbing sphere. We can short-circuit this calculation by noting that a version of Gauss's law holds here, which tells us that the net flux through a surface surrounding a set of sources is proportional to the total strength of those sources. In this case, the total strength is equal to the strength of the original source plus that of the image source, which is the strength of the original source multiplied by $1 - r_0/R$. The fraction of the total number of walkers that emanate from the source that also escape from the sphere is $(R - r_0)/R$.

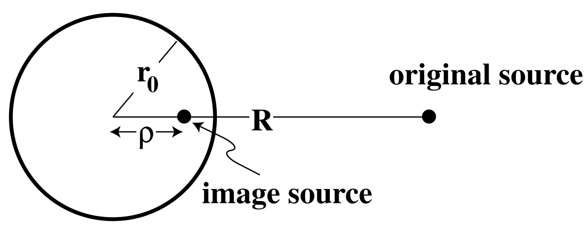

Figure 6: The source and the image source in the case of an absorbing sphere.

What we have also achieved here is a derivation of the probability of escape by a three-dimensional walker from a spherical region in the vicinity of its point of origin.

The analogy with capacitance

There is a mathematical connection between an absorbing surface into which matter diffuses from a distance and the element of a capacitor . Because of the relationship between the concentration and the electrostatic potential, we can imagine an analogy in which the surface is that of a conductor, surrounded by a spherical shell some distance away. If the potential difference between the two is $\Delta\phi$, and the charge on the inner surface is Q, then the capacitance of the system is $c = Q/\Delta\phi$. The connection between charge and the electrostatic potential is $\rho(\vec{r}) = -4\pi\nabla^2\phi(\vec{r})$. The total charge on the inner surface is, then as given by Gauss's law

$$Q = -\frac{1}{4\pi} \int \vec{\nabla}\phi(\vec{r}) \cdot d\vec{S} \tag{38}$$

Making use of the relationships we've already established between electrostatic quantities and those in steady state diffusion, we can state that the following holds

$$\frac{-\int \vec{j}(\vec{r}) \cdot d\vec{S}}{c_\infty} = 4\pi\beta C \tag{39}$$

where c_∞ is the concentration of walkers far away from the absorbing surface and C is the capacitance of a capacitor consisting of the absorbing surface surrounded, at a great distance, by a spherical shell. See Figure 7. For

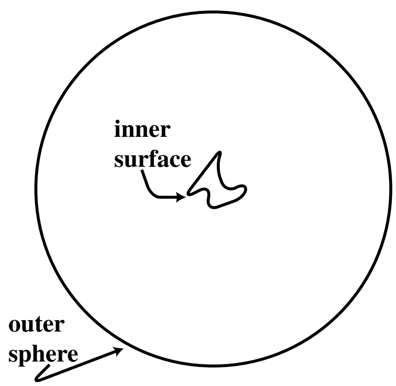

Figure 7: The capacitor consisting of an inner surface surrounded by a spherical shell. The radius of the surrounding shell is much greater than the size of the inner surface.

reference, recall that the capacitance of a sphere is given by

$$C_{\text{sphere}} = r_0 \tag{40}$$

where r_0 is the sphere's radius. This and (39) yields (37) for the total current absorbed by the sphere, where we have replaced c_0 by c_∞.

A sphere covered with receptors

This allows us to consider what happens if the nutrients are not absorbed uniformly throughout the sphere. Suppose, instead, that the sphere has a number of absorbing sites, or receptors, distributed across its surface. Imagine that there are n of those receptors, and that the radius of a given site is a. We'll also assume that $na \ll r_0$, where r_0 is the sphere's radius. This means that the total surface area accounted for by the receptors is a small fraction of the surface area of the sphere. Let's represent this collection of receptors as a network of small conducting surfaces, arranged in the shape of a spherical shell. This network is utilized as one of the elements in a capacitor . What is the capacitance of the resulting capacitor?

First, note that the distance between the receptors is the order of $r_0/\sqrt{n}$. Then, notice that the potential a distance r away from the sphere, where $r \gg r_0/\sqrt{n}$, is going to be the same as the electrostatic potential generated by a uniform distribution of the receptors, smeared out over the sphere. This is because at such a distance, the difference between a set of discrete charge and a uniformly distributed charge is negligible, as far as the electrostatic potential goes. If a charge of Q/n is placed on each receptor, then the electrostatic potential of this array of charges goes as $Q/(r + r_0)$. The electrostatic potential near the sphere is, then, well approximated by Q/r_0. This means that the capacitance of the spherical arrangement is substantially equal to the capacitance of a uniform sphere. Making use of the electrostatic analogy, we find that the collection of receptors will absorb nutrients at the same rate as if the entire surface of the sphere were a receptor.

We can be a little more explicit about the potential immediately above the surface of the network. The electrostatic potential right next to one of the small components of the network due to the charge carried by that component will go as Q/na, because each of the components carries a charge equal to Q/n, and each has an effective size equal to a. On the other hand, the potential due to all the other components will be essentially the same as if the charges on them were uniformly distributed over the surface of the sphere. This potential is equal to $Q(n-1)/nr_0$. If n is large enough that $na \gg r_0$, which is possible for sufficiently large n, since all we require is that $a \ll r/\sqrt{n}$, the potential is dominated by the second contribution, which, in the limit of large n, goes to Q/r_0. The potential at a point near the surface of the sphere that is far away from one of the small components compared to its size will be absolutely dominated by the second term. Thus, to a very good approximation, the electrostatic potential in the immediate vicinity of the network is the same as the electrostatic potential right next to a sphere carrying a uniform charge equal to Q.

For a more extended discussion of the issued addressed in the last two sections see the references [Berg, 1993] and [Berg and Purcell, 1977].

Finally, the generating function

At the outset I made reference to the utility of the generating function. Now it is time to actually talk about the object. Briefly, the generating function, $G(z;\vec{x},\vec{y})$ has the same relationship to the function $C(N;\vec{x},\vec{y})$ that the grand partition function in statistical mechanics has the partition function. Here, explicitly, is the expression for the random walk generating function

$$G(z;\vec{x},\vec{y}) = \sum_{N=0}^{\infty} C(N;\vec{x},\vec{y})z^N \tag{41}$$

The quantity z plays the role of the fugacity, $e^{\beta\mu}$ in statistical mechanics. The function $G(z;\vec{x},\vec{y})$ is called the generating function because when it is expanded in a power series in z the coefficients of that series are the functions $C(N;\vec{x},\vec{y})$. Of course, this relationship is pretty obvious, given the definition of $G(z;\vec{x},\vec{y})$.

Thus, the generating function encapsulates information about the statistical properties of random walks of all lengths. However, what makes the generating function so absolutely valuable is the fact that its determination is in many cases so much more straightforward than is the case for functions describing random walks with a fixed number of steps. In this respect, it possesses the same advantages as the grand partition function in many case, and example being quantum statistical mechanics, the natural approach to which is in the grand canonical ensemble.

To see how recourse to the generating function simplifies our consideration of random walk statistics, consider the recursion relation (3). Let's multiply both sides of this equation by Z^{N+1} and sum from $N=0$ to ∞. Then, we find

$$\begin{aligned}
\sum_{N=0}^{\infty} Z^{N+1}C(N+1;\vec{x},\vec{y}) &= \sum_{M=0}^{\infty} z^M C(M;\vec{x},\vec{y}) - C(0;\vec{x},\vec{y}) \\
&= G(z;\vec{x}.\vec{y}) - \delta_{\vec{x},\vec{y}} \\
&= z\sum_{N=0}^{\infty} z^N \sum_{\vec{w}_i} C(N;\vec{x},\vec{y})
\end{aligned}$$

$$= z \sum_{\vec{w}_i} G(z, \vec{x}, \vec{w}_i) \tag{42}$$

In deriving the expression on the second line of (42), we made use of the fact that the the number of zero step walks starting at $\vec{x}$ and ending at $\vec{y}$ is equal to one if the two locations are identical and is zero otherwise. The relationship that can be abstracted from (42) is

$$G(z; \vec{x}, \vec{y}) = z \sum_{\vec{w}_i} G(z; \vec{x}, \vec{w}_i) + \delta_{\vec{x},\vec{y}} \tag{43}$$

The recursion relation becomes an equation that is algebraic in the variable z. To further reduce it, we will focus on the situation in which there are no boundaries or any other object providing a reference point in space, which means that translational invariance holds. The generating function will then depend on the positions x and y only through their difference. In other words we can write the generating function in the form $G(z; \vec{y} - \vec{x})$. If we introduce the Fourier transformed generating function $g(z; \vec{q})$, given by

$$g(z; \vec{q}) = \sum_{\vec{x}} e^{-i\vec{q}\cdot(\vec{y}-\vec{x})} G(z; \vec{y} - \vec{x}) \tag{44}$$

then, multiplying Eq. (43) by $e^{-i\vec{q}\cdot(\vec{y}-\vec{x})}$ and summing over $\vec{x}$, we obtain

$$\begin{aligned} g(z; \vec{q}) &= \sum_{\vec{x}} e^{-i\vec{q}\cdot(\vec{y}-\vec{x})} G(z; \vec{y} - \vec{x}) \\ &= z \sum_{\vec{x}} \sum_{\vec{w}_i} e^{-i\vec{q}\cdot(\vec{y}-\vec{x})} G(z; \vec{w}_i - \vec{x}) + \sum_{\vec{x}} e^{-i\vec{q}\cdot(\vec{y}-\vec{x})} \delta_{\vec{x},\vec{y}} \\ &= z \sum_{\vec{w}_i} e^{i\vec{q}\cdot(\vec{w}_i-\vec{y})} \sum_{x} e^{-i\vec{q}\cdot(\vec{w}_i-\vec{x})} G(z; \vec{w}_i - \vec{x}) + 1 \\ &= z \sum_{\vec{w}_i} e^{i\vec{q}\cdot(\vec{w}_i-\vec{y})} g(z; \vec{q}) + 1 \\ &= z\chi(\vec{q}) g(z; \vec{q}) + 1 \end{aligned} \tag{45}$$

The function $\chi(\vec{q})$ in the last line of (45) is shorthand for the quantity $\sum_{\vec{w}_i} e^{i\vec{q}\cdot(\vec{w}_i-\vec{y})}$. Again, we abstract an equation for $g(z; \vec{q})$ from the several lines of (45). The equation is

$$g(z; \vec{q}) = z\chi(\vec{q}) g(z; \vec{q}) + 1 \tag{46}$$

The solution is easy. It is

$$g(z;\vec{q}) = \frac{1}{1 - z\chi(\vec{q})} \tag{47}$$

To extract the generating function in real space, we evaluate the Fourier transform of the function $g(z;\vec{q})$. We find

$$\begin{aligned} G(z;\vec{y}-\vec{x}) &\propto \int g(z;\vec{q}) e^{i\vec{q}\cdot(\vec{y}-\vec{x})} d^d q \\ &= \int \frac{e^{i\vec{q}\cdot(\vec{y}-\vec{x})}}{1 - z\chi(\vec{q})} d^d q \end{aligned} \tag{48}$$

Note that I have left the dimensionality of the integration in (48) unspecified. This because our general result is valid in all dimensions. The proportionality sign and the lack of explicit indications of the range of integration over the wave vector variable $\vec{q}$ arises from the lack of specification with regard to the exact conditions under which the random walker moves. Once that specification is supplied (Is the walker confined to the vertices of a lattice? If so, what kind of lattice? If not, what kind of randomness is there in the walk—in direction only or both in direction and in the length of the step?), both the overall multiplying constant and the range of $\vec{q}$-integration follows.

Given the generating function, we are now in a position to extract, if we so desire, the statistical properties of the N-step walk. Given that we've gone to the trouble to derive the expression on the last line of (48) for the generating function, let's see what we get when we do the power series expansion in z of it. Fortunately the first step is easy. We have

$$\frac{1}{1 - z\chi(\vec{q})} = \sum_{n=0}^{\infty} z^n \chi(\vec{q})^n \tag{49}$$

Performing the expansion in the integrand in the last line of (48), we end up with the following result for $C(N;\vec{x},\vec{y})$.

$$C(N;\vec{x},\vec{y}) \propto \int e^{i\vec{q}\cdot(\vec{y}-\vec{x})} \chi(\vec{q})^N d^d q \tag{50}$$

The exact result will depend on the exact form of the function $\chi(\vec{q})$. However, we can extract the important properties of the generating function by expanding that function as a power series in $\vec{q}$. To make contact with earlier results, we will look at a walker that is, again restricted to the vertices of a cubic lattice. The distance between neighboring points on that lattice will be a, as previously specified. Then

$$\begin{aligned}
&\sum_{\vec{w}_i} e^{i\vec{q}\cdot(\vec{w}_i-\vec{y})} \\
&\quad = e^{iaq_1}+e^{-iaq_1}+e^{iaq_2}+e^{-iaq_2}+e^{iaq_3}+e^{-iaq_3} \\
&\quad = 6-a^2(q_1^2+q_2^2+q_3^2)+O(q_l^4)
\end{aligned} \tag{51}$$

We now recast the integral leading to the generating function and make use of the expansion in (51).

$$\begin{aligned}
&C(N;\vec{x},\vec{y}) \\
&\quad \propto \int e^{i\vec{q}\cdot(\vec{y}-\vec{x})} e^{N\ln\chi(\vec{q})} d^3q \\
&\quad = \int e^{i\vec{q}\cdot(\vec{y}-\vec{x})} \exp\left[N\ln\left(6-a^2(q_1^2+q_2^2+q_3^2)\right)\right] d^3q \\
&\quad = \int e^{i\vec{q}\cdot(\vec{y}-\vec{x})} \exp\left[N\ln 6-\frac{Na^2}{6}|\vec{q}|^2\right] d^3q \\
&\quad = 6^N\left(\frac{6\pi}{Na^2}\right)^{3/2} e^{-3|\vec{y}-\vec{x}|^2/2Na^2}
\end{aligned} \tag{52}$$

Compare this to (24). We have the number of walks to within an overall multiplicative constant, which, after all, was left as an open item.

Now, let's turn our attention to the properties of the generating function itself. As it turns out, the most important properties are determined by the low order terms in the expansion of $\chi(\vec{q})$. In other words, it suffices to consider the quantity

$$\begin{aligned}
\frac{1}{1-z(\chi(0)+q^2\chi''(0))} &\equiv \frac{1}{1-(z/z_c)+Azq^2} \\
&\rightarrow \frac{1}{1-z/z_c+z_cAq^2}
\end{aligned} \tag{53}$$

We can, for instance, make use of the last line of (53) to reconstruct the generating function in real space:

$$G(z;\vec{x},\vec{y}) \propto \int \frac{e^{-\vec{q}\cdot(\vec{y}-\vec{x})}}{1-z/z_c+z_cAq^2} d^dq \tag{54}$$

We can perform the integral in (54) in three dimensions. We have

$$\begin{aligned} G(z;\vec{x},\vec{y}) &\propto 2\pi \int q^2\, dq \int d\theta \frac{e^{iq|\vec{y}-\vec{x}|\cos\theta}\sin\theta}{1-z/z_c+z_cAq^2} \\ &= \frac{4\pi}{|\vec{y}-\vec{x}|}\int_0^\infty \frac{\sin(q|\vec{y}-\vec{x}|)}{1-z/z_c+z_cAq^2} q dq \\ &= \frac{2\pi^2}{Az_c}\frac{e^{-\sqrt{1-z/z_c}\ |\vec{y}-\vec{x}|/\sqrt{z_cA}}}{|\vec{y}-\vec{x}|} \end{aligned} \tag{55}$$

The last line of (55) applies for $|\vec{y}-\vec{x}|$ not too small. The fact that the expression diverges as $\vec{y}\to\vec{x}$ is an artifact of our approximations and of the absence of a restriction on the integration over $\vec{q}$. One thing to note is that, aside from the divergent term—which is absent if we do the integration properly—the leading order contribution to the generating function as $\vec{y}\to\vec{x}$ goes as $\sqrt{z_c-z}$. This allows us to work out the dependence on N of the number of walks that return to the point from which they started. First, though, a digression on the art of extracting the coefficient of z^N in the power series of a function.

Extraction of coefficient of z^N in the power series expansion of a function with various singularities

In the cases of interest to us, the generating function displays singular structure as a function of the variable z in the vicinity of a "critical value," z_c. Here is a summary of the ways in which the coefficients of z^N behave for $N \gg 1$ in the cases of various possible singularities.

A simple pole

Let's start with one of the simplest examples of a function with an infinite power series expansion in z: $f(z)=1/(z_c-z)$. If $\mid z \mid < \mid z_c \mid$, we have

$$\begin{aligned} \frac{1}{z_c-z} &= \frac{1}{z_c}\left[1+\frac{z}{z_c}+\left(\frac{z}{z_c}\right)^2+\cdots\right] \\ &= \frac{1}{z_c}\sum_{n=0}^{\infty}\left(\frac{z}{z_c}\right)^n, \end{aligned} \tag{56}$$

so the coefficient of z^N is $z_c^{-(N+1)}$.

Two or more simple poles

Now, suppose z_c and z_d are both real, positive numbers and $z_c < z_d$. Furthermore, let

$$f(z) = \frac{a}{z_c - z} + \frac{b}{z_d - z}. \tag{57}$$

Then, if z is suficiently small($z < z_c$),

$$f(z) = \frac{a}{z_c} \sum_{n=0}^{\infty} \left(\frac{z}{z_c} \right)^n + \frac{b}{z_d} \sum_{n=0}^{\infty} \left(\frac{z}{z_d} \right)^n, \tag{58}$$

so the coefficient of z^N is $c_N = a z_c^{-(N+1)} + b z_d^{-(N+1)}$.

We can also write

$$c_N = a z_c^{-(N+1)} \left[1 + \frac{b}{a} \left(\frac{z_c}{z_d} \right)^{N+1} \right].$$

Now, let $z_c = z_d(1 - \Delta)$, where $\Delta > 0$. Then

$$\begin{aligned} c_N &= a z_c^{-(N+1)} \left[1 + \frac{b}{a} (1 - \Delta)^{N+1} \right] \\ &= a z_c^{-(N+1)} \left[1 + \frac{b}{a} e^{(N+1) \ln(1-\Delta)} \right] \\ &= a z_c^{-(N+1)} \left[1 + \frac{b}{a} e^{-\delta(N+1)} \right], \end{aligned} \tag{59}$$

where $\delta = -\ln(1 - \Delta)$ and $\delta > 0$. As N gets larger and larger the second term in brackets in (59) vanishes exponentially. Thus, for very large N the coefficient of z^N in $a/(z_c - z) + b/(z_d - z)$ is essentially equal to the coefficient of $a/(z_c - z)$. We will eventually generalize this result as follows:

If the functions $f_a(z)$ and $f_b(z)$ have poles or branch points at z_a and z_b, respectively, and if $z_b > z_a > 0$ (z_a and z_b both real), then, when N is large, the coefficient of z^N in $Af_a(z) + Bf_b(z)$ is, for all practical purposes, equal to the coefficient of z^N in $Af_a(z)$.

Higher Order Poles and Branch Points

What about the more general case $f(z) = (z_c - z)^{-\alpha}$, where the exponent α need not be an integer? One way of finding the coefficient of z^N is to use the binomial expansion formula. Another way is the use the following identity:

$$\int_0^\infty t^A e^{-xt}\,dt = x^{-A-1}\Gamma(A+1), \tag{60}$$

where $\Gamma(A)$ is the gamma function. When A is an integer, n, $\Gamma(n+1) = n!$. With the use of (60) we have

$$(z_c - z)^{-\alpha} = \frac{1}{\Gamma(\alpha)} \int_o^\infty t^{\alpha-1} e^{-t(z_c - z)}\,dt. \tag{61}$$

To find the coefficient ofz^N in $(z_c - z)^{-\alpha}$ we expand the right hand side of the above equation with respect to z. The coefficient of z^N in that expansion is

$$\begin{aligned}\frac{1}{\Gamma(\alpha)}\frac{1}{N!}\int_0^\infty t^{\alpha-1+N} e^{-tz_c}\,dt &= \frac{1}{\Gamma(\alpha)}\frac{1}{N!} z_c^{-(N+\alpha)}\Gamma(\alpha+N) \\ &= \frac{\Gamma(\alpha+N)}{\Gamma(\alpha)\Gamma(N+1)} z_c^{-(N+\alpha)}. \end{aligned} \tag{62}$$

Now, we use Stirling's formula for the gamma function of a large argument

$$\Gamma(N) = e^{(N-1)\ln(N-1)-(N-1)} \qquad N \gg 1 \tag{63}$$

When N is large, the coefficient of interest is

$$\begin{aligned}\frac{z_c^{-N-\alpha}}{\Gamma(\alpha)} e^{(\alpha+N-1)\ln(\alpha+N-1)-(\alpha+N-1)-N\,\ln N + N} &= \frac{z_c^{-N-\alpha}}{\Gamma(\alpha)} e^{(\alpha-1)\ln(N)} \\ &= \frac{z_c^{-N-\alpha}}{\Gamma(\alpha)} N^{\alpha-1} \end{aligned} \tag{64}$$

Logarithmic Singularities

One more complication: suppose the function is of the form $-(z_c - z)^{-\alpha}\ln(z_c - z)$. We obtain the coefficient of z^N by noting that this function is just

$\frac{d}{d\alpha}(z_c - z)^{-\alpha}$. Taking the derivative with respect to α of the last term in the equation above, we have for the desired coefficient

$$\begin{aligned}
\frac{d}{d\alpha}\frac{z_c^{-N-\alpha}}{\Gamma(\alpha)}N^{\alpha-1} &= \ln(z_c)\frac{z_c^{-N-\alpha}N^{\alpha-1}}{\Gamma(\alpha)} - \frac{\Gamma'(\alpha)z_c^{-N-\alpha}}{\Gamma(\alpha)^2}N^{\alpha-1} + \ln(N)\frac{z_c^{-N-\alpha}N^{\alpha-1}}{\Gamma(\alpha)} \\
&= \ln(N)\frac{z_c^{-N-\alpha}}{\Gamma(\alpha)}N^{\alpha-1}\left(1 + O\left(\frac{1}{\ln(N)}\right)\right) \qquad (65)
\end{aligned}$$

By the same token, we can find the coefficient of z^N in $-(z_c - z)^{-\alpha}/\ln(z_c - z)$ by extracting the coefficient of z^N in the integral

$$\int_{-\alpha}^{\infty}(z_c - z)^y \, dy, \qquad (66)$$

Using (64) to find the coefficient of z^N in the integrand, one is left with

$$\begin{aligned}
\int_{-\alpha}^{\infty}\frac{z_c^{-N+z}}{\Gamma(-z)}N^{z-1}\,dz &= -\left.\frac{N^{z-1}}{\ln N}\frac{z_c^{-N+z}}{\Gamma(-z)}\right|_{-\alpha}^{\infty} - \frac{1}{\ln N}\int_{-\alpha}^{\infty}N^{z-1}\frac{d}{dz}\left(\frac{z_c^{-N+z}}{\Gamma(-z)}\right)dz \\
&= \frac{N^{\alpha-1}z_c^{-N-\alpha}}{\ln(N)\Gamma(\alpha)}\left(1 + O\left(\frac{1}{\ln N}\right)\right). \qquad (67)
\end{aligned}$$

The first equality in (67) results from an integration by parts. An additional integration by parts establishes the second equality.

Back to the generating function

Now, let's see how the generating function depends on the difference $z_c - z$ when we let the end point approach the location from which the walker starts. We will look this behavior in various dimensions. We start by setting $\vec{y} = \vec{x}$. Then,

$$\begin{aligned}
G(z; \vec{x} = \vec{y}) &\propto \int \frac{d^d q}{1 - z/z_c + \mathcal{A}q^2} \\
&\propto \int \frac{q^{d-1}\,dq}{1 - z/z_c + \mathcal{A}q^2} \qquad (68)
\end{aligned}$$

To simplify expressions, I have replaced the combination $z_c A$ by $\mathcal{A}$ in the denominator. There is a quick and dirty way to extract the singular dependence of the integral on the last line of (68) on $z_c - z$, and that is to scale the combination out of the integrand. We do this with a change of integration variables, replacing q by $(1 - z/z_c)^{1/2} q'$. This leaves us with the integral

$$\begin{aligned} \int \frac{(1 - z/z_c)^{d/2} {q'}^{d-1}\, dq'}{(1 - z/z_c) + \mathcal{A}{q'}^2} &= (1 - z/z_c)^{(d-2)/2} \int \frac{{q'}^{d-1}\, dq'}{1 + \mathcal{A}{q'}^2} \\ &= (1 - z/z_c)^{(d-2)/2}\, \mathcal{C} \end{aligned} \tag{69}$$

Our ability to successfully scale $(1 - z/z_c)$ out of the integral requires that we not have to worry about limits on the integration. By and large, this does not prove to be a problem, except in the special case $d - 2$. In two dimensions, we have the following integral to perform

$$\begin{aligned} \int_0^Q \frac{q\, dq}{1 - z/z_c + \mathcal{A}q^2} &= \frac{1}{2\mathcal{A}} \ln\left[1 - z/z_c + \mathcal{A}q^2\right]\Big|_0^Q \\ &= \frac{1}{2\mathcal{A}} \left\{\ln\left[1 - z/z_c + \ln Q^2\right] - \ln\left[1 - z/z_c\right]\right\} \end{aligned} \tag{70}$$

A couple of points. First, I put an upper limit, Q, on the integral, because otherwise it is not convergent. The second is that the value of Q is actually irrelevant to the singularity of interest, which arises from the contribution from the lower limit at $Q = 0$.

Now, making use of the methods described on pages 23–26, we find that the coefficient of z^N in the expansion of the generating function $G(z; \vec{x} = \vec{y})$ goes as $N^{-d/2}$. I should say that we would not have had to go through the indirect route of the generating function to obtain that result. We could have obtained the same result by generalizing the integral over $\vec{q}$ in (22) to d dimensions.

Recurrence

One of the important properties of a random walk is related to the likelihood that a walker will visit a particular site. An issue related to this property has to do with the question of *recurrence*, which is to say, the problem of calculating the likelihood that a walker returns to its point of origin. As it turns out, the answer to this question depends importantly on the dimension in which the random walk is executed. Here we will work out an expression that allows us to answer the question of recurrence, and, when properly extended, to work out the number of different sites visited by a random walker. First, though, an altered version of the generating function

A new generating function

A useful—but apparently little known[2]—quantity enables one obtain some key results with remarkably little effort. This quantity is an expanded version of the generating function we've been utilizing, and it refers to a walk that may or may not visit a special site. Suppose the quantity $C(N, M; \vec{x}, \vec{y}, \vec{w})$ is the number of N-step walks that start at the location $\vec{x}$, end at the location $\vec{y}$ and visit the site at location $\vec{w}$ exactly M times in in the process of getting from $\vec{x}$ to $\vec{y}$. The quantity of interest is

$$C'(N, t; \vec{x}, \vec{y}, \vec{w}) = \sum_{M=0}^{\infty} C(N, M; \vec{x}, \vec{y}, \vec{w})(1-t)^M \tag{71}$$

Clearly, terms in the sum on the right-hand side of the above equation for which $M > N + 1$ will not count, as there is no walk that visits a site more times than it leaves footprints. That is $C(N, M; \vec{x}, \vec{y}, \vec{w}) = 0$ if $M > N + 1$. We obtain the coefficients of the power series expansion in $(1-t)^n$ that produces this generating function in the standard way. It is easy to show that

$$C(N, M; \vec{x}, \vec{y}, \vec{w}) = (-1)^M \frac{1}{M!} \frac{d^M}{dt^M} C'(N, t; \vec{x}, \vec{y}, \vec{w}) \Big|_{t=1} \tag{72}$$

Note that in this case the value to which the expansion parameter is set is not zero, but rather one.

Derivation of the new generating function

We derive the new generating function by introducing a weighting factor. The weighting factor W has the following form for an N-step walk that visits the site s_i at the i^{th} step

$$W = \prod_{i=1}^{N} w(s_i) \tag{73}$$

where factor $w(s_i)$ is given by

$$w(s_i) = 1 - t\delta_{s_i, S} \tag{74}$$

[2]Little known among practicing solid state physicists, that is.

Here, S is the special site of interest. The overall weighting factor for a given walk is then

$$\prod_{i=1}^{N}(1 - t\delta_{s_i,S}) \tag{75}$$

Suppose $t = 1$. Then, the weighting factor will have the effect of excluding any walk that visits the special site S; all other walks will have a weighting factor of one. This means that if we multiply all walks by the weighting factor above, set $t = 1$ and sum, we will obtain the number of walks that never visit the site S. In the case of N-step walks that start at $\vec{x}$ and end up at $\vec{y}$, this is just $C(N, 0; \vec{x}, \vec{y}, \vec{w})$, where $\vec{w}$ is the position vector of the site S. Suppose we take the derivative of the weighted sum with respect to t, and then set $t = 1$. In that case, we will end up with -1 times the number of walks that visit the site only once. Next, take the n^{th} derivative of the weighted sum over walks with respect to t, multiply by $1/n!$, and then set $t = 1$. This yields $(-1)^n$ times the number of walks that visit the special site exactly n times. This is because each derivative generates a factor equal to $-\delta_{s_j,S}$ and all terms that "escape" the derivative become $(1 - \delta_{s_k,S})$ when $t = 1$. The factor $1/n!$ compensates for the $n!$ ways in which the n derivatives with respect to t operate on the product in (75).

Now, we can evaluate the weighted walk by expanding the weighting factor, (75), in powers of t.[3] At first order we generate the quantity

$$-t\sum_{i=1}^{N}\delta_{s_i,S} \tag{76}$$

When walks are multiplied by this weighting factor and summed we end up with $-t$ times the sum of all N-step walks that visit the site S at one step, with no restriction on what happens either before or after that step. At second order in the expansion we have

$$t^2\sum_{i=1}^{N}\sum_{j=1}^{i-1}\delta_{s_i,S}\delta_{s_j,S} \tag{77}$$

When walks are multiplied by this second-order weighting factor and summed, we end up with t^2 times the sum of all N-step walks that visit the site S

[3] We are thus treating t as if it were a small quantity and expanding in it. This technique will be used later for a different expansion parameter in the case of self-avoiding walks, in which case we will generate a virial expansion.

twice with no restriction on what happens before, after or between those two visitations. A graphical representation for the expansion in t of the new generating function is shown in Fig. 8. If the starting and end-point of the

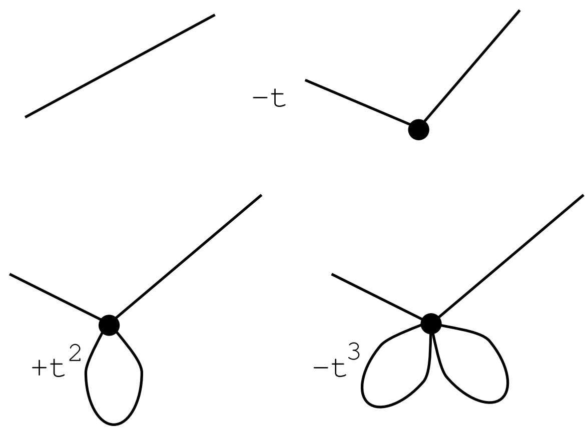

Figure 8: The graphical representation of the virial expansion of the generating function defined in (71). The large dots in the diagrams lie at the location $\vec{w}$.

walk are fixed, and if the site in question is at the location v, then the sum in Fig. 8 is given by

$$C(N;\vec{x},\vec{y}) - t\sum_{N_1+N_2=N} C(N_1;\vec{x},\vec{w})C(N_2;\vec{w},\vec{y}) \\ +t^2 \sum_{N_1+N_2+N_3=N, N_2\geq 1} C(N_1;\vec{x},\vec{w})C(N_2;\vec{w},\vec{w})C(N_3;\vec{w},\vec{y}) + \cdots \quad (78)$$

The inequality that applies to N_2 in the sum above simply requires the walker to take at least one step before revisiting the site at $\vec{w}$. Otherwise, we would count zero step "walks" in the sum.

Now, we take the step of multiplying our new function by z^N and summing. This has the effect of removing the convolution over the N_i's, and we obtain

$$\begin{aligned} G(z,t;\vec{x},\vec{y},\vec{w}) &= \sum_{N=0}^{\infty} z^N C'(N,t;\vec{x},\vec{y},\vec{w}) \\ &= G(z;\vec{x},\vec{y}) - tG(z;\vec{x},\vec{w})G(z;\vec{w},\vec{y}) \end{aligned}$$

$$
\begin{aligned}
& +t^2 G(z;\vec{x},\vec{w})G_1(z;\vec{w},\vec{w})G(z;\vec{w},\vec{y}) + \cdots \\
= \quad & G(z;\vec{x},\vec{y}) - t\frac{G(z;\vec{x},\vec{w})G(z;\vec{w},\vec{y})}{1 - tG_1(z;\vec{w},\vec{w})}
\end{aligned} \tag{79}
$$

The subscript 1 in $G_1(z;\vec{w},\vec{w})$ indicates that it is a generating function for walks of at least one step.

The quantity

$$
\begin{aligned}
& (-1)^M \frac{1}{M!}\frac{d^M}{dt^M} G(z,t;\vec{x},\vec{y},\vec{w})\Big|_{t=1} \\
= \quad & (-1)^M \frac{1}{M!}\frac{d^M}{dt^M}\left[G(z;\vec{x},\vec{y}) - t\frac{G(z;\vec{x},\vec{w})G(z;\vec{w},\vec{y})}{1 - tG_1(z;\vec{w},\vec{w})}\right]\Bigg|_{t=1}
\end{aligned} \tag{80}
$$

is, then, the generating function for all walks that start at $\vec{x}$, end up at $\vec{y}$ and visit the site at $\vec{w}$ exactly M times.

Dimensionality and the Probability of Recurrence

Our result allows us to determine whether or not a random walk is **recurrent**. If it is, then almost all long random walks that start out at a given point will revisit that point. If it is not, then only a finite fraction of those walks do so, and the walk is called **transient**. Recurrent walks are also referred to as "persistent." Pólya [Pólya, 1919] was the first to demonstrate that walks occuring in one and two dimensions return to their starting point with absolute certainty, if they consist of an infinite number of steps and that in higher dimensions the walker has a non-zero probability of never revisiting its starting point, no matter how long its walk. Let's see what (79) tells us about the recurrence of random walks on a lattice. We want to know how many of the walks that start out at $\vec{x}$ revisit their point of origin, so we set $\vec{w}$ in (79) equal to $\vec{x}$. The generating function takes the form

$$
G(z;\vec{x}-\vec{y}) - t\frac{G_1(z;0)G(z;\vec{x}-\vec{y})}{1+tG_1(z;0)} = \frac{G(z;\vec{x}-\vec{y})}{1+tG_1(z;0)}. \tag{81}
$$

The reason for the subscript 1 in the numerator of the second term on the left hand side of (81) is that we want to count only those walks that take at least one step from the starting point at x before revisiting that point. Otherwise, we count walks that "revisit" their point of origin after zero steps.

To find out how many N-step walk start out at $\vec{x}$ and end up at $\vec{y}$, never having revisited $\vec{x}$, we need to calculate the coefficient of z^N in the function

$$\frac{G(z;\vec{x}-\vec{y})}{1+G_1(z;0)} = \frac{G(z;\vec{x}-\vec{y})}{G(z;0)}. \tag{82}$$

The right hand side of the equality in (82) follows from the fact that the contribution to the generating function $G(z;0)$ of walks consisting of no steps is exactly one, by convention.

Let's be even less restrictive and ask how many of the walks that start out at $\vec{x}$ and end up *anywhere* never revisit the starting point $\vec{x}$. We simply sum the expression above over all possible end-points $\vec{y}$—excluding $\vec{x}$—and see what we have. Using the relation between $G(z;\vec{x}-\vec{y})$ and its spatial fourier transform, $g(z;\vec{q})$ we have

$$\begin{aligned} \sum_{\vec{y}\neq\vec{x}} \frac{G(z;\vec{x}-\vec{y})}{G(z;0)} &= \frac{g(z;0)}{G(z;0)} - \frac{G(z;0)}{G(z;0)} \\ &= \frac{g(z;0)}{G(z;0)} - 1, \end{aligned} \tag{83}$$

where we have used the identity

$$g(z,0) = \sum_{\vec{y}} G(z,\vec{x}-\vec{y}) \tag{84}$$

for the fourier coefficient $g(z,\vec{q})$. From Chapter 2, we know that

$$\begin{aligned} g(z,\vec{q}=0) &= \frac{1}{1-z\chi(\vec{q}=0)} \\ &\equiv \frac{1}{1-z/z_c} \end{aligned} \tag{85}$$

The last line of (85) serves as a definition of the quantity z_c. This tells us that the number of N-step walks that start out at $\vec{x}$ and end up anywhere is the coefficient of z^N in $(1-z/z_c)^{-1}$, while the number of walks that start at $\vec{x}$ and end up anywhere, not having ever revisited the point of origin, $\vec{x}$, is the coefficient of z^N in

$$\frac{z_c}{z_c - z}\frac{1}{G(z;0)} \tag{86}$$

As it turns out, the z-dependence of the generating function $G(z;0)$ in two dimensions or less is different in a very important respect from its behavior in three and higher dimensions. This will lead to fundamentally different results for the "recurrence" of walks in two and one dimensions from what we will find in the case of three dimensional walks.

The Notion and Quantification of Shape

Shape is an intuitively accessible notion. We organize visual information in terms of shapes, and the shape of an object represents one of the first of its qualities referred to in an informal descriptive rendering of it. While our language presents us with a wide repertoire of verbal images for the approximate portrayal of the shape of a physical entity ("round," "oblong," "crescent," "stellate" ...) the precise characterization of a shape, in terms of a number, or set of numbers, has remained elusive. This is with good reason. It is well-known to mathematicians that the class consisting of the set of all curves is a higher order of infinity than the set of all real numbers. This means that there can be no one-to-one correspondence between curves and real numbers. As shapes, intuitively at least, bear a conceptual relationship to curves, it is plausible that the set of all shapes dwarfs in magnitude the set of real numbers, or of finite sets of real numbers.

On the other hand, if one is willing to content oneself with a general paradigm for the measurement of shape, there are ways of quantifying it in terms of numbers that have a certain descriptive and predictive utility. In fact, the numerical specification of shapes has acquired a certain urgency of late, in light of the widespread use of computer imaging and the concommitant focus on the development of codes for the creation and manipulation of pictorial quantities.

In this Chapter, we will look at different ways of characterizing and measuring the shape of a random walk. We will focus on one particular method, based on calculations of the width of the distribution of steps about the "center of mass" of the walk. The particular quantity studied is the radius of gyration tensor, and the shape of the polymer is quantified in terms of the eigenvalues of this tensor, termed the principal radii of gyration of the walk. We will look at a particular combination of the principal radii of gyration that provides information with respect to the deviation from spherical symmetry of the shape of the walk. It will turn out that shape as a concept is, as one might expect, a bit elusive. For one thing, there is no generic “shape” for a random walk. However, statistical statements can be made, with regard to the probability that a walk takes on a particular shape, at least as characterized by the principal radii of gyration. In addition, there is one limit in which the shape of the trail left by a walker is fixed and predictable. That is the limit of a walker in an infinite dimensional space ($d = \infty$). We will discuss the construction of an expansion about that limit, the $1/d$-expansion. This expansion yields the shape distribution of a random walker's trail when the walker wanders in a high spatial dimension environment. As we will see, this expansion is—at least for some puroposes—respectably accurate in three dimensions.

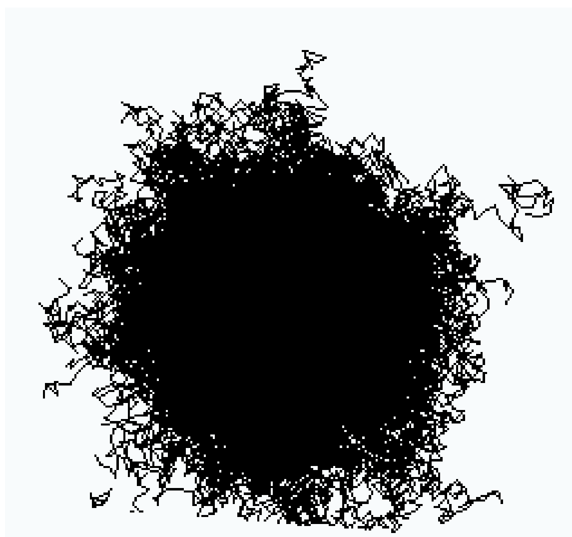

Figure 9: A “cloud” consisting of the paths of 1,000 random walkers, each of which has taken 100 steps from a common point of origin.

Anisotropy of a random walk

When we talk about the distribution of points visited by a random walker, we generally do so in the context of ensemble averages. That is, we ask *on average* how many walks visit a given point. Looking at things this way can obscure the detailed structure of a given random walk. For example, if we are interested in how many time a given point at location $\vec{r}_1$ is visited by a walker that starts out at the location $\vec{r}_0$, we find, after suitable averaging, that the answer depends only on the distance between those points in space, $|\vec{r}_1 - \vec{r}_0|$. This is true because for every walker that tends to go off in one direction there will be another walker that ends up going in the opposite direction. The statistical distribution of places visited is rotationally symmetric about the point of origin. In other words, the totality of walkers in the ensemble create a "cloud" that is spherically symmetric. Figure 9 shows just such a cloud, which consists of the paths of 1,000 random walkers each of whom has taken 100 steps from a common point of origin. The near spherical symmetry of the cloud is evident from the figure.

This result of averaging obscures the fact that a given random walk can be quite anisotropic spatially. Figure 10 is a stereographic pair of images of a single 1,000-step random walk. The elongated nature of the walk shown in this figure is not a statistical anomaly. Figure 11 shows several examples of 1,000-step walks. Note that not one of those walks is reminiscent of the cloud of walkers shown in Figure 9.

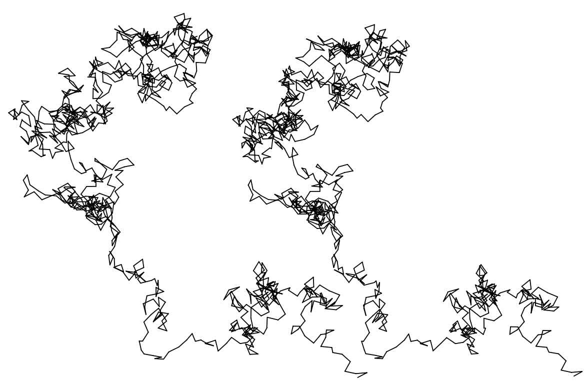

Figure 10: Stereographic pair of images of a 1,000 step three-dimensional random walk.

On the other hand, as Figure 11 makes abundantly clear, no typical, or definitive, shape can be assigned to a random walk. How, then, to quantify the shape of a walk?

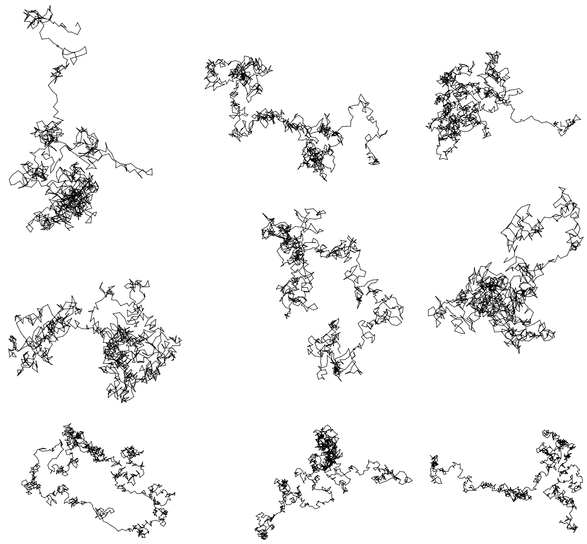

Figure 11: Several examples of a 1,000-step random walk.

Measures of the shape of a walk

There are in the literature a number of algorithm for the characterization of the shape of an object [Bookstein, 1978, Costa and Cesar, 2001]. Here, we choose one that is particularly well-suited to our needs. We construct a moment-of-inertia-like tensor (See Supplement 1 at the end of this chapter). By diagonalizing this tensor we are able to extract numbers that quantify the linear "size" of the walk in various directions, particularly in the directions in which it has the greatest linear extent and the direction in which it is most compact. For a visualization of this, see Figure 12, in which the extensions in both directions of a two-dimensional random walk is illustrated. The thick lines indicate the directions in which random walk has the greatest and the smallest extension, as determined by the tensor that we are about to introduce. Note that these two lines provide a quantitative representation of both the overall orientation of the walk and of its spatial anisotropy—that is, degree to which the shape of the walker's path differs from that of a sphere. As we will see, the amount of anisotropy exhibited by the walks in Figures 10 11 and 12 is not at all atypical. [4]

[4] For a characterization of the anistropy of a random walker using the notion of spans, see [Weiss and Rubin, 1976]. Here, our approach will be somewhat different.

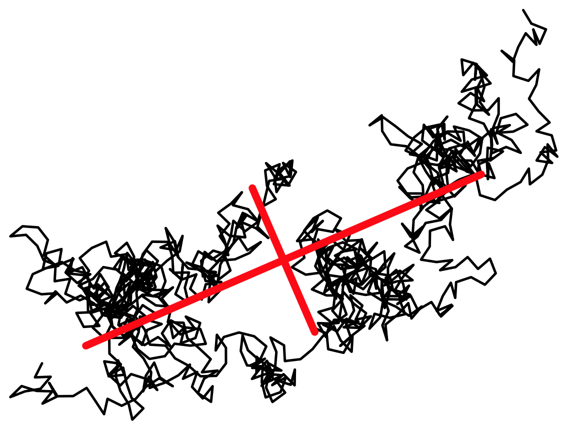

Figure 12: The anisotropic nature of a 1,000-step two-dimensional walker. The red lines indicate the directions in which its linear extent is the greatest and the smallest. The lines also run parallel to the eigenvectors of the matrix defined in Eqs. (87)–(89). The point of intersection of those two lines is the "center of gravity" of the walk.

The radius of gyration tensor

The tensor that we are about to define is also utilized to determine the rotational inertia of a three-dimensional object. Supplement 1 at the end of this chapter reviews its use in that context. What this means is that the results to be derived here are relevant to the rotational motion of an object that mimics the form of the path followed by a random walker, assuming that the constituents of this object have an inertial mass, that they are uniformly distributed along the path it imitates, and that the object is, itself, rigid.

Here is how the tensor is constructed [Solc and Stockmayer, 1971]. Given the location, $\vec{r}_i$ $(1 \leq i \leq N)$, of each step of a walker in d dimensions that has left N footprints, we construct a d dimensional tensor, $\overleftrightarrow{T}$ with entries

$$T_{kl} = \frac{1}{N} \sum_{j=1}^{N} \left(r_{jk} - \langle r_k \rangle\right) \left(r_{jl} - \langle r_l \rangle\right) \tag{87}$$

Here, r_{jk} is the k^{th} component of the position vector of the j^{th} step, and $\langle r_k \rangle$ is the average of the k^{th} component of the locations of the steps of the walker:

$$\langle r_k \rangle = \frac{1}{N} \sum_{j=1}^{N} r_{jk} \tag{88}$$

For example, a walker in two dimensions has **radius of gyration tensor** $\overleftrightarrow{T}$ with the following form

$$\overleftrightarrow{T} = \begin{pmatrix} \frac{1}{N}\sum_{j=1}^{N}\left(x_j - \langle x \rangle\right)^2 & \frac{1}{N}\sum_{j=1}^{N}\left(x_j - \langle x \rangle\right)\left(y_j - \langle y \rangle\right) \\ \frac{1}{N}\sum_{j=1}^{N}\left(x_j - \langle x \rangle\right)\left(y_j - \langle y \rangle\right) & \frac{1}{N}\sum_{j=1}^{N}\left(y_j - \langle y \rangle\right)^2 \end{pmatrix} \tag{89}$$

The eigenvectors and eigenvalues of this tensor quantify the linear dimensions of the walker—its girth—in various directions. The eigenvectors point in the direction in which this span is maximized, and the direction in which it is minimized. The eigenvalues tell us how extended the walk is in those extremal directions. In fact, the lines in Fig. 12 lie along the directions in which those two eigenvectors point. The lengths of those lines are directly proportional to the eigenvalues of the matrix $\overleftrightarrow{T}$ appropriate to the walk in that figure.

For a discussion of the relationship between the eigenvectors and eigenvalues of $\overleftrightarrow{T}$ and the maximal and minimal spans of a walk see the section beginning on page 47 in Supplement 1 at the end of this chapter.

Eigenvalues of the matrix $\overleftrightarrow{T}$: the asphericity of a random walk

The eigenvalues of the matrix $\overleftrightarrow{T}$ are the squares of the **principal radii of gyration**, R_i, of the object in question. They are essentially the mean square deviations of the steps of the walker from the "center of gravity" of the walk. In Fig 12 the walk's center of gravity lies at the point of intersection of the two thick lines, each of which lie in the direction of the eigenvectors of the matrix $\overleftrightarrow{T}$ for that walk. This means that diagonalized, the matrix $\overleftrightarrow{T}$ takes the form

$$\overleftrightarrow{T} = \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix}$$

$$\equiv \begin{pmatrix} R_1^2 & 0 & 0 \\ 0 & R_2^2 & 0 \\ 0 & 0 & R_3^2 \end{pmatrix} \tag{90}$$

The relative magnitudes of the eigenvalues of the radius of gyration tensor $\overleftrightarrow{T}$ then tell us to what extent the object in question has a shape that differs from that of a sphere. Clearly if all R_i^2's in (90) are equal, then the linear span of the object will be the same in all directions, and it is reasonable to attribute a kind of spherical symmetry to it. However, if, for example, $R_1^2 \gg R_2^2, R_3^2$, which means that R_1 is significantly larger than R_2 and R_3, then the object can be thought of as greatly elongated, and not at all spherical.

The eigenvalues of an object's radius of gyration tensor are invariant with respect to the overall orientation of the object. That is, a rotation of the object will not change those eigenvalues. On the other hand, the tensor itself does change as the object is rotated. If the brackets $\langle \cdots \rangle_r$ stand for averaging with respect to overall orientation, then the average $\langle R_i^2 \rangle_r$ is just the same as R_i^2. On the other hand, performing the same average over $\overleftrightarrow{T}$ produces a matrix altered by the averaging process. In fact, it is pretty straightforward to argue that $\langle (x - \langle x \rangle)(y - \langle y \rangle) \rangle_r$ will average to zero, while $\langle (x - \langle x \rangle)^2 \rangle_r = \langle (y - \langle y \rangle)^2 \rangle_r = \langle (z - \langle z \rangle)^2 \rangle_r$ This means that

$$\langle \overleftrightarrow{T} \rangle = \begin{pmatrix} \bar{T} & 0 & 0 \\ 0 & \bar{T} & 0 \\ 0 & 0 & \bar{T} \end{pmatrix} \tag{91}$$

The eigenvalues of this matrix are clearly all equal to $\bar{T}$. In averaging the radius of gyration tensor, we are performing the kind of ensemble average that destroys information regarding the non-spherical shape of the object in question. This clearly means an informative characterization of the shape of the random walk is not contained in the averaged radius of gyration tensor.

We can, nevertheless extract useful shape information by averaging quantities that are directly derivable from the radius of gyration matrix. What we need to do is use quantities that are invariant with respect to rotations and reflections in space (the matrix is automatically invariant with respect to translations). All of these quantities are directly related to the eigenvalues of the matrix. In the case of a three dimensional matrix there are three independent invariants. One choice of those three is

$$\mathrm{Tr}\, \overleftrightarrow{T} = T_{11} + T_{22} + T_{33}$$

$$= R_1^2 + R_2^2 + R_3^2 \tag{92}$$

$$\mathrm{Tr}\,\overleftrightarrow{T}^2 = (R_1^2)^2 + (R_2^2)^2 + (R_3^2)^2 \tag{93}$$

$$\mathrm{Tr}\,\overleftrightarrow{T}^3 = (R_1^2)^3 + (R_2^2)^3 + (R_3^2)^3 \tag{94}$$

Another well-known invariant of the tensor, its determinant is obtained as follows

$$\begin{aligned}
\mathrm{Det}\,\overleftrightarrow{T} &= R_1^2 R_2^2 R_3^2 \\
&= \frac{1}{6}\Big[\left(R_1^2 + R_2^2 + R_3^2\right)^3 + 2\left((R_1^2)^3 + (R_2^2)^3 + (R_3^2)^3\right) \\
&\quad -3\left(R_1^2 + R_2^2 + R_3^2\right)\left((R_1^2)^2 + (R_2^2)^2 + (R_3^2)^2\right)\Big] \\
&= \frac{1}{6}\left[\left(\mathrm{Tr}\,\overleftrightarrow{T}\right)^3 + 2\,\mathrm{Tr}\,\overleftrightarrow{T}^3 - 3\,\mathrm{Tr}\,\overleftrightarrow{T}\,\mathrm{Tr}\,\overleftrightarrow{T}^2\right]
\end{aligned} \tag{95}$$

Now, it is possible to average the three invariants defined in Eqs. (92)–(94). These averages retain important information regarding the devation from spherical symmetry of the shape of the “average” random walk. Consider, for example, the following combination of eigenvalues

$$\begin{aligned}
&\left(R_1^2 - R_2^2\right)^2 + \left(R_1^2 - R_3^2\right)^2 + \left(R_2^2 - R_3^2\right)^2 \\
&= 3\left((R_1^2)^2 + (R_2^2)^2 + (R_3^2)^2\right) - \left(R_1^2 + R_2^2 + R_3^2\right)^2 \\
&= 3\,\mathrm{Tr}\,\overleftrightarrow{T}^2 - \left(\mathrm{Tr}\,\overleftrightarrow{T}\right)^2
\end{aligned} \tag{96}$$

Both sides of this equation can be averaged over all orientations of an object, and, given the fact that they are invariants with respect to translation, rotation and reflection, they will remain unchanged. In the case of the random walk, this means that if we average the last line of (96) over an ensemble of walkers we are left with a quantity that tells us something about the differences between the various principal radii of gyration. That is, we find out how different the shape a random walk is, on the average, from that of a sphere.

To construct a quantity that interpolates between zero when all principal radii of gyration are equal and one when one of the R_i's is much greater than the others we will divide by

$$2\langle(\sum_{i=1}^{3} R_i^2)^2\rangle = 2\langle \mathrm{Tr}\,\overleftrightarrow{T}\rangle^2 \tag{97}$$

We can, in fact, generalize this quantity and define the mean **asphericity**, A_d, of d-dimensional random walks as follows [Aronovitz and Nelson, 1986, Theodorou and Suter, 1985, Rudnick and Gaspari, 1986]:

$$A_d = \frac{\sum_{i>j}^{d} \langle (R_i^2 - R_j^2)^2 \rangle}{(d-1)\langle (\sum_{i=1}^{d} R_i^2)^2 \rangle} \tag{98}$$

The numerator of (98) can be rewritten as follows:

$$\begin{aligned} &\langle \left(R_1^2 - R_2^2\right)^2 + \left(R_1^2 - R_3^2\right)^2 + \cdots \left(R_{d-1}^2 - R_d^2\right)^2 \rangle \\ = \ & d\,\mathrm{Tr}\langle \overleftrightarrow{T}^2 \rangle - \langle \left(\mathrm{Tr}\, \overleftrightarrow{T}\right)^2 \rangle \\ = \ & d(d-1)\left(\langle T_{11}^2 \rangle - \langle T_{11} T_{22} \rangle\right) + d^2(d-1)\langle T_{12}^2 \rangle \end{aligned} \tag{99}$$

The last line of (99) follows from the equations for the trace of a tensor and of its square. It also follows from the fact that $\langle T_{11}^2 \rangle = \langle T_{22}^2 \rangle = \cdots \langle T_{dd}^2 \rangle$, and similar equalities for $\langle T_{ii} T_{jj} \rangle$ and $\langle T_{ij}^2 \rangle$. The denominator of the last line of (98) can be reduced in the same way, leading to the following expression for the asphericity:

$$\begin{aligned} A_d &= \frac{d(d-1)\left(\langle T_{11}^2 \rangle - \langle T_{11} T_{22} \rangle\right) + d^2(d-1)\langle T_{12}^2 \rangle}{d(d-1)\langle T_{11}^2 \rangle + d(d-1)^2 \langle T_{11} T_{22} \rangle} \\ &= \frac{\left(\langle T_{11}^2 \rangle - \langle T_{11} T_{22} \rangle\right) + d\langle T_{12}^2 \rangle}{\langle T_{11}^2 \rangle + (d-1)\langle T_{11} T_{22} \rangle} \end{aligned} \tag{100}$$

The calculation of the asphericity reduces to the problem of determining the average values of powers of the entries in the radius of gyration tensor. The details, which are a bit involved, are described later on in this lecture. The end-result of the calculation is the following general expression for the mean asphericity of a d-dimensional random walk:

$$A_d = \frac{4 + 2d}{4 + 5d} \tag{101}$$

The three-dimensional walk has a mean asphericity of 10/19, or a little more than a half, so in this sense the three-dimensional walk is, on the average, somewhere between an isotropic object and a highly elongated one.

Of course the notion of the mean asphericity of a random walk does not necessarily imply that there is a characteristic shape for three dimensional

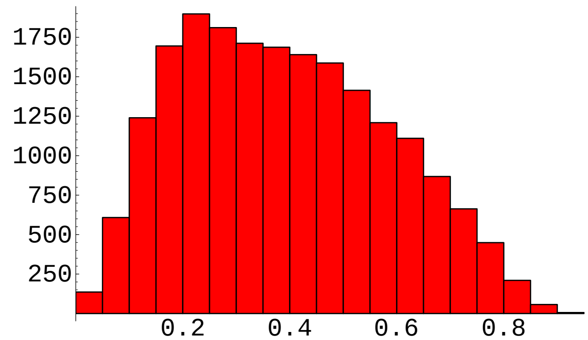

Figure 13: The distribution of the individual asphericities of 20,000 three-dimensional 100 step walks.

walks. Given the examples depicted in Fig. 11, it seems much more likely that random walks come in a wide variety of shapes and that a quantity such as the mean asphericity provides a very broad-brush characterization of that property of random walks. Figure 13 illustrates this point. It is a histogram of the distribution of the individual asphericities of 20,000 three-dimensional walks, each comprised of 100 steps. Note that the distribution spans the range from 0 to 1, and that no narrow region dominates.

It is also important to note that what is presented in (101) is not, strictly speaking, the average of the individual asphericities of the walks, which is given by

$$A'_d = \left\langle \frac{\sum_{i<j} \left(R_i^2 - R_j^2\right)^2}{(d-1)\sum_{k=1}^{N} R_k^2} \right\rangle \tag{102}$$

This quantity can also be found exactly in the case of the ordinary d-dimensional walk. The analytical result for this quantity is [Diehl and Eisenregler, 1989]

$$A'_d = \frac{d}{4}\left[3 + \frac{4}{d} - \frac{d}{2} M_{d/2}\right] \tag{103}$$

where

$$M_p = \int_0^\infty x^{p+1} \sinh^{-p} x \; dx \tag{104}$$

In three dimensions, $A'_d = 0.394274\ldots$. The average of the individual asphericities is somewhat smaller than the mean asphericity.

Shape of a self-avoiding random walk

Work on the shape of a self-avoiding walk has been performed [Aronovitz and Nelson, 1986]. The calculation is based on an expansion in the difference between the dimensionality in which the walk takes place and an " upper critical dimensionality," equal to four. The quantity $\epsilon = 4 - d$ is the expansion parameter. To first order in ϵ

$$A_d = \frac{2d+4}{5d+4} + 0.008\epsilon \tag{105}$$

The main conclusion to be gleaned from this result is that self-avoidance plays a non-trivial, but far from decisive, role in the shape of a random walk. [5]

Principal radii of gyration and rotational motion

Recall Newton's second law:

$$\vec{F} = \frac{d\vec{p}}{dt} \tag{106}$$

Here, $\vec{F}$ is the applied force and $\vec{p}$ is the linear momentum of the particle or collection of particles to which that force is applied. When the system undergoing the change in motion is a single particle, $\vec{p} = m\vec{v}$, where $\vec{v}$ is the particle's velocity. Now, assume that we have a system of particles. Newton's second law, as it refers to each point particle, is, then

$$\vec{F}_l = m_l \frac{d\vec{v}_l}{dt} \tag{107}$$

where l is the subscript that identifies the particle. If we sum up these equations we end up with (106), where F is the net external force (internal forces cancel because of Newton's third law), and $\vec{p}$ is the total momentum:

$$\vec{p} = \sum_l m_l \vec{v}_l \tag{108}$$

[5] Notice that the first term on the right hand side of (105) has not been expanded about $d = 4$. This is a (minor) violation of the spirit of the expansion in $\epsilon = 4 - d$, which does not materially affect the conclusion stated above.

So far, so good. This is all pretty elementary. Now, let's focus on rotational motion. We derive Newton's second law, as it applies to rotational motion, by taking the cross product of the position vectors $\vec{r}_l$ with the corresponding equation in the set (107). Defining the total torque $\vec{\tau}$ as the sum of the $\vec{r}_l \times \vec{F}_l$'s, we end up with the equation

$$\begin{aligned} \vec{\tau} &= \sum_l m_l \vec{r}_l \times \frac{d\vec{v}_l}{dt} \\ &= \frac{d}{dt} \sum_l m_l \vec{r}_l \times \vec{v}_l \\ &\equiv \frac{d\vec{L}}{dt} \end{aligned} \tag{109}$$

The last two lines of (109) constitute a definition of the angular momentum, $\vec{L}$ of a system of point particles. Note that the precise definition of angular momentum depends on the origin with respect to which the position of each particle is defined. It is often convenient to place the origin in at the center of mass of the set of particles. If the internal force between each pair of particles is along the line joining them, then the internally generated torques cancel, and the total torque, $\vec{\tau}$, is entirely due to external forces.

Now, suppose that the motion of the system is entirely rotational, about some point $\vec{R}$. Then,

$$\vec{v}_l = \vec{\omega} \times \left(\vec{r}_l - \vec{R} \right) \tag{110}$$

Here, $\vec{\omega}$ is the angular velocity of the system of particles. See Figure 14. Now, we can choose $\vec{R}$ as the center of our system of coordinates, so that $\vec{r}_l - \vec{R}$ is replaced by $\vec{r}_l$. In this case, the angular momentum becomes

$$\sum_l m_l \vec{r}_l \times (\vec{\omega} \times \vec{r}_l) \tag{111}$$

We can rewrite the above relationship with the use of the standard identity for the triple product:

$$\vec{L} = \sum_l m_l \left(\vec{\omega} \left(\vec{r}_l \cdot \vec{r}_l \right) - \vec{r}_l \left(\vec{r}_l \cdot \vec{\omega} \right) \right) \tag{112}$$

Suppose, now, we define the matrix $\overleftrightarrow{T}$ as follows:

$$T_{ij} = \sum_l m_l r_{l,i} r_{l,j} \tag{113}$$

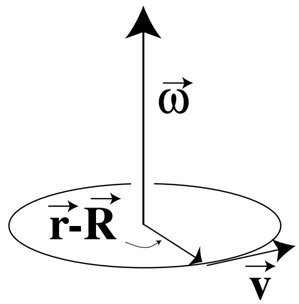

Figure 14: The angular velocity, $\vec{\omega}$, and its relation to the velocity,$\vec{v}$, of a particle.

Then, the relationship between $\vec{L}$ and $\vec{\omega}$ is

$$\vec{L} = \mathrm{Tr}\,\overleftrightarrow{T}\,\vec{\omega} - \overleftrightarrow{T}\cdot\vec{\omega} \tag{114}$$

Defining

$$\overleftrightarrow{C} = \overleftrightarrow{T} - \overleftrightarrow{I}\,\mathrm{Tr}\,\overleftrightarrow{T} \tag{115}$$

where $\overleftrightarrow{I}$ is the identity operator we find that

$$\vec{L} = -\overleftrightarrow{C}\cdot\vec{\omega} \tag{116}$$

Note that the trace of the operator $\overleftrightarrow{C}$ has a trace equal to twice the trace of $\overleftrightarrow{T}$. This is because the trace of the identity operator is three. The matrix $\overleftrightarrow{C}$ is the moment-of-inertia matrix. The fact that the angular velocity and the angular momentum are not parallel is just one of the complications of rotational motion.

Now, because the matrix $\overleftrightarrow{T}$ is real and symmetric, we know that it has real (in fact, positive) eigenvalues. Those eigenvalues have a name. They are known as the principal radii of gyration, R_i^2. If $\vec{\omega}$ points in the same direction as the eigenvector of one of them, say R_1^2, then the angular momentum and the angular velocity point in the same direction, and the relationship between the two becomes

$$\vec{L} = \left(R_2^2 + R_3^2\right)\vec{\omega} \tag{117}$$

This is because $\mathrm{Tr}\,\overleftrightarrow{T} = R_1^2 + R_2^2 + R_3^2$, while $\overleftrightarrow{T}\cdot\vec{\omega} = R_1^2\vec{\omega}$.

The eigenvalues of the tensor $\overleftrightarrow{T}$ can also be used as a measure of the extent to which the system of particles possesses spherical symmetry, at least in terms of rotational motion. If all the egenvalues are equal, then the system has approximately the same weighted extent. In fact, in this case, $\vec{L}$ is always parallel to $\vec{\omega}$.

Now imagine that all the masses, m_l, are equal to one. Then, the matrix measures the extent to which the particles are in a spherically symmetric distribution. While equality of the principal radii of gyration is not equivalent to spherical symmetry, it provides a very useful quantitative measure of that property, and of departure from it.

We can construct our tensor, $\overleftrightarrow{Q}$, as follows

$$\overleftrightarrow{Q}=\overleftrightarrow{T}-\frac{1}{3}\overleftrightarrow{I}\ \mathrm{Tr}\ \overleftrightarrow{T} \tag{118}$$

The trace of this matrix is equal to zero, and, if all the principal radii of gyration are the same, then the diagonalized form of this matrix has all entries equal to zero.

Position vectors transform under rotations about the center of mass as follows

$$r'_k = \sum_l R_{kl} r_l \tag{119}$$

where R_{kl} are the elements of the rotation matrix. This matrix has the property that its transpose is also its inverse. That is

$$\overleftrightarrow{R}\cdot\overleftrightarrow{R}^T=\overleftrightarrow{I} \tag{120}$$

A matrix whose transpose is also its inverse is known as an orthogonal matrix. Then, the matrix $\overleftrightarrow{T}$ with elements going as $r_l r_k$ transforms as follows

$$\begin{aligned} T'_{k_1k_2} &= \sum_{l_1,l_2} R_{k_1l_1} T_{l_1l_2} R_{k_2l_2} \\ &= \sum_{l_1,l_2} R_{k_1l_1} T_{l_1l_2} R^T_{l_2k_2} \\ &= \sum_{l_1,l_2} R_{k_1l_1} T_{l_1l_2} R^{-1}_{l_2k_2} \end{aligned} \tag{121}$$

or, in shorthand,

$$\overleftrightarrow{T}'=\overleftrightarrow{R}\cdot\overleftrightarrow{T}\cdot\overleftrightarrow{R}^{-1} \tag{122}$$

The same relationship clearly holds for the tensor $\overleftrightarrow{Q}$. The demonstration that traces of powers of this tensor are invariant under rotations follows from this equation for the way in which rotations give rise to changes in $\overleftrightarrow{Q}$.

Just a little bit more on the meaning of the operator $\overleftrightarrow{T}$.

Suppose we are interested in finding the direction in which an object is has the greatest spatial extent. We start by assuming a vector $\vec{n}$, which points

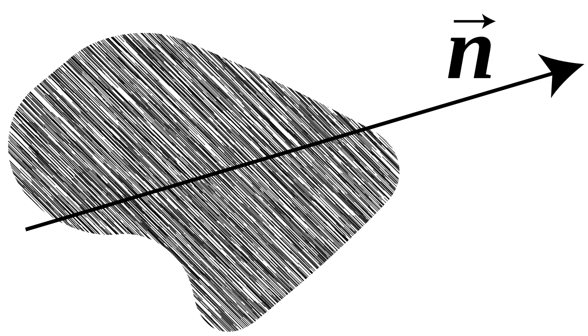

Figure 15: Looking for the direction in which an object has the greatest spatial extent.

along the direction of interest. We will set the length of the vector at unity. See figure 15. Then the extent of the object in the direction established by $\vec{n}$ is

$$\sum_l (\vec{r}_l \cdot \vec{n})^2 = \sum_l \sum_{i,j} n_i r_{l,i} r_{l,j} n_j = \vec{n} \cdot \overleftrightarrow{T} \cdot \vec{n} \tag{123}$$

Remember that the position vectors are drawn with their tails at the center of mass of the object. If we wish to extremize the above quantity with respect to $\vec{n}$, subject to the condition that its length is held constant, we take the derivative with respect to each component of $\vec{n}$ of the expression below

$$\vec{n} \cdot \overleftrightarrow{T} \cdot \vec{n} - \lambda \vec{n} \cdot \vec{n} \tag{124}$$

The quantity λ in (124) is a Lagrange multiplier. The extremum equation easily reduces to

$$\overleftrightarrow{T} \cdot \vec{n} = \lambda \vec{n} \tag{125}$$

That is, in order to find the direction of greatest (or least) extent of the object, we solve the eigenvalue equation of the operator $\overleftrightarrow{T}$. The largest eigenvalue is the greatest extent, as defined by (123), with $\vec{n}$ chosen to extremize the quantity.[6] The smallest extent, similarly defined, is given by the smallest eigenvalue of $\overleftrightarrow{T}$.

Calculations for the mean asphericity

The average $\langle T_{11} \rangle$

First, we slightly recast the general expression for the mean asphericity

$$A_d = \frac{\left(\frac{\langle T_{11}^2 \rangle}{\langle T_{12}^2 \rangle} - \frac{\langle T_{11} T_{22} \rangle}{\langle T_{12}^2 \rangle} \right) + d}{\frac{\langle T_{11}^2 \rangle}{\langle T_{11} T_{22} \rangle} + d - 1} \tag{126}$$

This means that to calculate the mean aspericity we need to find ratios of averages, rather than the averages themselves. This simplifies our task a bit.

Although the averages that we have to perform in order to arrive at a numerical result for the asphericity of the random walk involve squares of entries in the radius of gyration tensor, or products of two entries, it is useful to look at the average of a single element of that tensor, lying along the diagonal. Eventually, we will perform this calculation in another way when we develop an expansion in $1/d$ for the principal radii of gyration. However, we will start out by showing how the calculation can be done with the use of the generating functions that have proven so useful in the study of random walk statistics. As a first step, we recast the expression for the entries T_{kl}: [7]

$$T_{kl} \;\; = \;\; \frac{1}{N} \sum_{j=1}^{N} \left(r_{jk} - \langle r_k \rangle \right) \left(r_{jl} - \langle r_l \rangle \right)$$

[6]In other words, the extremizing choice for the vector $\vec{n}$ is the eigenvector of the operator $\overleftrightarrow{T}$ with the largest eigenvalue.

[7]Here, we make no distinction between N and $N+1$

$$= \frac{1}{2N^2} \sum_{i=1}^{N} \sum_{j=1}^{N} (r_{ik} - r_{jk})(r_{il} - r_{jl}) \tag{127}$$

The first line in the above equation is a recapitulation of (87). The second line can be established by inspection. Consider, now the average

$$\langle T_{11} \rangle = \frac{1}{2N^2} \sum_{i=1}^{N} \sum_{j=1}^{N} \langle (x_i - x_j)^2 \rangle \tag{128}$$

We have reverted here to the notation appropriate to a three-dimensional walk, and replaced r_1 by x. The average in the sum on the right hand side of (128) is directly proportional to a function that can be graphically represented as shown in Fig. 16.

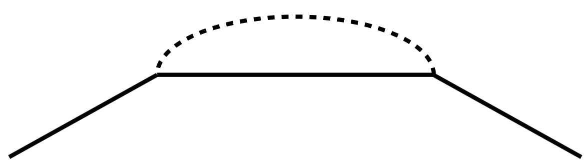

Figure 16: Graphical representation of $\langle (x_i - x_j)^2 \rangle$.

The dashed curve joins the i^{th} and j^{th} footprints on the walk. The solid lines stand for the walk that begins at the leftmost end of the three-line segment and ends at the righttmost point. There will, in general, be N_1 steps from the far left point to the leftmost vertex at which the dashed curve touches the line, N_2 steps in the central segment of the walk and N_3 steps in the far right segment of the walk. Subject to the overall constraint that the N_i's add up to the total number of steps in the walk, we sum over all values of N_1, N_2 and N_3. The evaluation of the sum represented by this diagram is most conveniently carried out in the grand canonical ensemble, with the use of the generating function. We seek the coefficient of z^{N-1} in the direct product

$$\frac{1}{2N^2} \times 2 \int d^d r_0 \int d^d r_2 \int d^d r_3 G(z; \vec{r}_1 - \vec{r}_0) G(z; \vec{r}_2 - \vec{r}_1) G(z; \vec{r}_3 - \vec{r}_2)(x_2 - x_1)^2 \tag{129}$$

The "missing" integration in (129), over $\vec{r}_1$, would yield a factor equal to the volume of the portion of space in which the random walk occurs. The factor of two multiplying the integral represent the two possible orderings of the indices i and j ($i > j$ and $i < j$). As the next step, we rewrite the generating functions in terms of their spatial Fourier transforms,

$$G(z;\vec{r}) = \frac{1}{(2\pi)^d} \int d^d k g(z;\vec{k}) e^{-\vec{k}\cdot\vec{r}} \tag{130}$$

Making use of this representation, we find that the expression in (129) reduces to

$$\frac{1}{N^2}\, g(z;\vec{k}) \left(-\frac{\partial^2}{\partial k_x^2} g(z;k) \right) g(z;\vec{k}) \Big|_{\vec{k}=0} \tag{131}$$

The second derivative follows from the identity

$$(x_1 - x_2)^2 e^{i\vec{k}\cdot(\vec{r}_1 - \vec{r}_2)} = -\frac{\partial^2}{\partial k_x^2} e^{i\vec{k}\cdot(\vec{r}_1 - \vec{r}_2)} \tag{132}$$

and an integration by parts. Once this identity and integration by parts has been implemented, the integrations over the $\vec{r}_i$'s produces Dirac delta functions in the k_i's, and we are immediately led to (131)

Now, in the case of a random walk in d dimensions, we can write

$$g(z;\vec{k}) = \frac{1}{1 - z z_c^{-1} + k^2 l^2/2d} \tag{133}$$

where l represents the mean distance covered by the walker in each step. This leaves us with the following result for the expression (131):

$$\frac{1}{N^2} \frac{l^2}{d} \frac{1}{(1 - z z_c^{-1})^4} \tag{134}$$

We now extract the coefficient of z^{N-1} in the power series expansion of (134).[8] This is straightforward given what we know about the process.[9] We find for this coefficient

$$\frac{1}{N^2} \frac{l^2}{d} z_c^{-(N-1)} \frac{(N+2)(N+1)N}{6} \approx \frac{1}{N^2} \frac{l^2}{d} z_c^{-(N-1)} \frac{N^3}{6} \tag{135}$$

[8]The relevant power is $N-1$ because there are $N-1$ steps in a walk that leaves N footprints

[9]See Supplement 3 in Chapter 2

This result is the desired value of $\langle T_{11} \rangle$, multiplied by the total number of random walks with $N-1$ steps. To obtain the average, we divide this by the total number of $N-1$-step walks, which is equal to the coefficient of z^{N-1} in

$$\begin{aligned} \int d^d r G(z;\vec{r}) &= g(z;\vec{k}=0) \\ &= \frac{1}{1-zz_c^{-1}} \end{aligned} \tag{136}$$

The coefficient in question is $z_c^{-(N-1)}$. We thus find

$$\langle T_{11} \rangle = N\frac{l^2}{6d} \tag{137}$$

The average of the trace of the tensor $\overleftrightarrow{T}$ is, by symmetry, equal to $d\langle T_{11} \rangle$. Given (137) we have

$$\langle \mathrm{Tr}\ \overleftrightarrow{T} \rangle = Nl^2/6 \tag{138}$$

The quantity above is also known as the mean radius of gyration .

Calculation of the asphericity

The quantities that contribute to the asphericity are $\langle T_{11}^2 \rangle$, $\langle T_{11}T_{22} \rangle$ and $\langle T_{12}^2 \rangle$. Again, reverting to standard cartesian notation we find

$$\begin{aligned} &\langle T_{11}^2 \rangle \\ &= \frac{1}{4N^4}\sum_{i=1}^{N}\sum_{j=1}^{N}\sum_{k=1}^{N}\sum_{l=1}^{N}\langle (x_i-x_j)^2\,(x_k-x_l)^2 \rangle \end{aligned} \tag{139}$$

Now, the graphical representation of the numerator in the expression leading to the desired average is a bit more complicated, in that there are three different forms, as shown in Fig. 17. The dotted curves are a stand-in for the differences $(x_m - x_n)^2$, and the three types of graphical representations correspond to the three "topologically distinct" possibilities for the sequence of the indices i, j, k, l in (139). The calculation proceeds along the same line as the one leading to a result for $\langle T_{11} \rangle$. As we can see from (98), the only information we need to extract from our calculation is the ratios $\langle T_{11}^2 \rangle / \langle T_{11}T_{22} \rangle$ and $\langle T_{11} \rangle / \langle T_{12} \rangle$. We will go over the determination of the average $\langle T_{11}^2 \rangle$ in detail. The other averages are determined in a similar way.

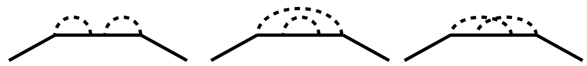

Figure 17: The three different forms of the graph involved in the calculation of $\langle T_{11}^2 \rangle$.

Determination of $\langle T_{11}^2 \rangle$.

We proceed diagram-by-diagram.

Diagram a

Here, the calculation proceeds as it did in the evaluation of $\langle T_{11} \rangle$. Taking second derivatives and performing integrations by parts, we are left with the following expression

$$\frac{1}{4N^4} \times 8\, g(z;\vec{k}) \left(\frac{\partial^2}{\partial k_x^2} g(z;\vec{k}) \right) g(z;\vec{k}) \left(\frac{\partial^2}{\partial k_x^2} g(z;\vec{k}) \right) g(z;\vec{k}) \Big|_{\vec{k}=0} \qquad (140)$$

The factor of 8 in the above expression counts the number of ways of constructing diagram a, exchanging end-points of the two dashed curves, and permuting the two curves amomng themselves. The quantity of interest is, of course, the coefficient of z^{N-1} in (140). We will defer the power series expansion in the fugacity z. Making use of (133) for the Fourier transformed generating function, we end up with the result

$$\frac{2}{N^4} \left(\frac{l^2}{d} \right)^2 \frac{1}{(1 - z z_c^{-1})^7} \qquad (141)$$

Diagram b

The evaluation of this diagram is a bit more involved. Utilizing the generating function in real space, we have the average of interest proportional to the following expression:

$$\begin{aligned} &\int d^d r_0 \int d^d r_1 \int d^d r_2 \int d^d r_3 \int d^d r_4 G\left(z; \vec{r}_1 - \vec{r}_0\right) \\ &\times G\left(z; \vec{r}_2 - \vec{r}_1\right) G\left(z; \vec{r}_3 - \vec{r}_2\right) G\left(z; \vec{r}_4 - \vec{r}_3\right) G\left(z; \vec{r}_5 - \vec{r}_4\right) \\ &\times \left(x_4 - x_1\right)^2 \left(x_3 - x_2\right)^2 \end{aligned} \qquad (142)$$

The next step is to express the generating functions in terms of their Fourier transforms. We end up with a product containg the factor

$$\begin{aligned}
&(x_4 - x_1)^2 (x_3 - x_2)^2 e^{i\vec{k}_0\cdot(\vec{r}_1-\vec{r}_0)} e^{i\vec{k}_1\cdot(\vec{r}_2-\vec{r}_1)} e^{i\vec{k}_2\cdot(\vec{r}_3-\vec{r}_2)} e^{i\vec{k}_3\cdot(\vec{r}_4-\vec{r}_3)} e^{i\vec{k}_4\cdot(\vec{r}_5-\vec{r}_4)} \\
&= \left(\frac{\partial}{\partial k_{2x}}\right)^2 \left(\frac{\partial}{\partial k_{1x}} + \frac{\partial}{\partial k_{2x}} + \frac{\partial}{\partial k_{3x}}\right)^2 e^{i\vec{k}_0\cdot(\vec{r}_1-\vec{r}_0)} e^{i\vec{k}_1\cdot(\vec{r}_2-\vec{r}_1)} e^{i\vec{k}_2\cdot(\vec{r}_3-\vec{r}_2)} \\
&\quad \times e^{i\vec{k}_3\cdot(\vec{r}_4-\vec{r}_3)} e^{i\vec{k}_4\cdot(\vec{r}_5-\vec{r}_4)}
\end{aligned} \tag{143}$$

After a series of integrations of parts in the variables $\vec{k}_i$ the derivatives above act on the Fourier transforms of the generating functions. The integrations over the $\vec{r}_l$'s produce delta functions, and we are left with the following result

$$\left(\frac{\partial}{\partial k_{2x}}\right)^2 \left(\frac{\partial}{\partial k_{1x}} + \frac{\partial}{\partial k_{2x}} + \frac{\partial}{\partial k_{3x}}\right)^2 g\left(z;\vec{k}_0\right) g\left(z;\vec{k}_1\right) g\left(z;\vec{k}_2\right) g\left(z;\vec{k}_3\right) g\left(z;\vec{k}_4\right)\Big|_{\vec{k}_0=\vec{k}_1=\vec{k}_2=\vec{k}_3=\vec{k}_4=0} \tag{144}$$

The polynomial expressions in the derivatives are now expanded, discarding in the process all terms that evaluate to zero when the $\vec{k}_i$'s are equal to zero.[10] This yields

$$\left(\frac{\partial^2}{\partial k_{1x}^2}\frac{\partial^2}{\partial k_{2x}^2} + \frac{\partial^2}{\partial k_{3x}^2}\frac{\partial^2}{\partial k_{2x}^2} + \frac{\partial^4}{\partial k_{2x}^4}\right) g\left(z;\vec{k}_0\right) g\left(z;\vec{k}_1\right) g\left(z;\vec{k}_2\right) g\left(z;\vec{k}_3\right) g\left(z;\vec{k}_4\right)\Big|_{\vec{k}_0=\vec{k}_1=\vec{k}_2=\vec{k}_3=\vec{k}_4=0} \tag{145}$$

The remainder of the calculation is fairly straightforward. Inserting combinatorial factors noted above and taking the appropriate derivatives of the generating function, we end up with the contribution

$$\frac{16}{N^4}\left(\frac{l^2}{d}\right)^2 \frac{1}{\left(1 - zz_c^{-1}\right)^7} \tag{146}$$

[10]The general operating principle is that any term that contains an odd-order derivative with respect to a k_{ix} will evaluate to zero.

Diagram c

In this case, the relevant identity is

$$\begin{aligned}
&(x_3-x_1)^2\,(x_4-x_2)^2\, e^{i\vec{k}_0\cdot(\vec{r}_1-\vec{r}_0)}e^{i\vec{k}_1\cdot(\vec{r}_2-\vec{r}_1)}e^{i\vec{k}_2\cdot(\vec{r}_3-\vec{r}_2)}e^{i\vec{k}_3\cdot(\vec{r}_4-\vec{r}_3)}e^{i\vec{k}_4\cdot(\vec{r}_5-\vec{r}_4)} \\
&= \left(\frac{\partial}{\partial k_{1x}}+\frac{\partial}{\partial k_{2x}}\right)^2\left(\frac{\partial}{\partial k_{2x}}+\frac{\partial}{\partial k_{3x}}\right)^2 e^{i\vec{k}_0\cdot(\vec{r}_1-\vec{r}_0)}e^{i\vec{k}_1\cdot(\vec{r}_2-\vec{r}_1)}e^{i\vec{k}_2\cdot(\vec{r}_3-\vec{r}_2)} \\
&\quad\times e^{i\vec{k}_3\cdot(\vec{r}_4-\vec{r}_3)}e^{i\vec{k}_4\cdot(\vec{r}_5-\vec{r}_4)} \qquad (147)
\end{aligned}$$

The same set of steps as outined immediately above leads to the following non-vanishing contributions to the diagram, combinatorial factors having been left out,

$$\begin{aligned}
&\left(\frac{\partial^2}{\partial k_{1x}^2}\frac{\partial^2}{\partial k_{2x}^2}+\frac{\partial^2}{\partial k_{3x}^2}\frac{\partial^2}{\partial k_{2x}^2}+\frac{\partial^2}{\partial k_{1x}^2}\frac{\partial^2}{\partial k_{3x}^2}+\frac{\partial^4}{\partial k_{2x}^4}\right) \\
&\quad g\left(z;\vec{k}_0\right)g\left(z;\vec{k}_1\right)g\left(z;\vec{k}_2\right)g\left(z;\vec{k}_3\right)g\left(z;\vec{k}_4\right)\Big|_{\vec{k}_0=\vec{k}_1=\vec{k}_2=\vec{k}_3=\vec{k}_4=0} \qquad (148)
\end{aligned}$$

Taking the derivatives indicated, evaluating the $\vec{k}_i=0$ limits and inserting the required combinatorial factors, we end up

$$\frac{18}{N^4}\left(\frac{l^2}{d}\right)^2\frac{1}{\left(1-zz_c^{-1}\right)^7} \qquad (149)$$

Summing all diagrams

Adding (141), (146) and (148), we end up with the following total contribution to the generating function yielding $\langle T_{11}^2\rangle$

$$\frac{36}{N^4}\left(\frac{l^2}{d}\right)^2\frac{1}{\left(1-zz_c^{-1}\right)^7} \qquad (150)$$

Actually, the generating function yields the numerator in a fraction. The denominator is the total number of $N-1$-step walks. However, as we are interested in ratios of averages, the common denominator is not important for our present purposes. For the same reason, we are not required to extract the coefficient of z^{N-1} in the power series expansion of (150), as that produces a common factor that cancels out when we evaluate ratios.

The ratios

The calculations of expressions contributing to $\langle T_{11}T_{22}\rangle$ and $\langle T_{12}^2\rangle$ proceed along the lines laid out above. For each of these averages, there are three contributions, corresponding to the three diagrams in Fig. 17. Carrying out the required computations, we find

$$\frac{\langle T_{11}^2\rangle}{\langle T_{11}T_{22}\rangle} = \frac{9}{5} \tag{151}$$

$$\frac{\langle T_{11}^2\rangle}{\langle T_{12}^2\rangle} = \frac{9}{2} \tag{152}$$

Inserting these results into the right of (126), we obtain (101) for the mean asphericity of a d-dimensional random walk. .ep

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