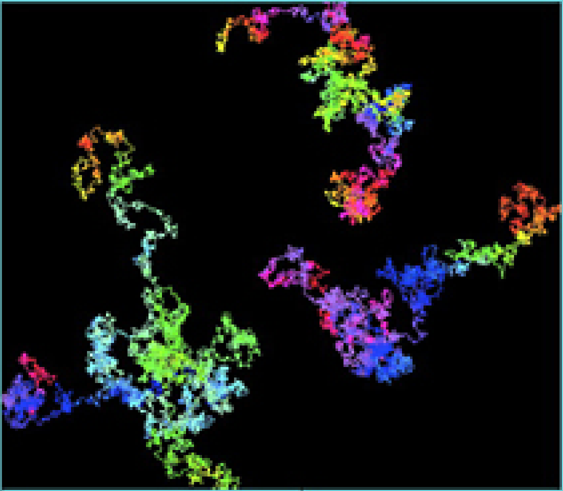
Elements of the Random Walk

An Introduction for Advanced Students and Researchers



Joseph Rudnick and George Gaspari

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ELEMENTS OF THE RANDOM WALK

An Introduction for Advanced Students and Researchers

Random walks have proven to be a useful model in understanding processes across a wide spectrum of scientific disciplines. *Elements of the Random Walk* is an introduction to some of the most powerful and general techniques used in the application of these ideas.

The mathematical construct that runs through the analysis of each of the topics covered in this book, and which therefore unifies the mathematical treatment, is the generating function. Although the reader is introduced to modern analytical tools, such as path integrals and field-theoretical formalism, the book is self-contained in that basic concepts are developed and relevant fundamental findings fully discussed. The book also provides an excellent introduction to frontier topics such as fractals, scaling and critical exponents, path integrals, application of the GLW Hamiltonian formalism, and renormalization group theory as they relate to the random walk problem. Mathematical background is provided in supplements at the end of each chapter, when appropriate.

This self-contained text will appeal to graduate students across science, engineering, and mathematics who need to understand the application of random walk techniques, as well as to established researchers.

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CAMBRIDGE
UNIVERSITY PRESS

CAMBRIDGE UNIVERSITY PRESS
Cambridge, New York, Melbourne, Madrid, Cape Town, Singapore, São Paulo

Cambridge University Press
The Edinburgh Building, Cambridge CB2 2RU, UK

Published in the United States of America by Cambridge University Press, New York

www.cambridge.org
Information on this title: www.cambridge.org/9780521828918

First published in print format 2004

ISBN-13 978-0-511-18934-0 eBook (Adobe Reader)
ISBN-10 0-511-18934-6 eBook (Adobe Reader)

ISBN-13 978-0-521-82891-8 hardback
ISBN-10 0-521-82891-0 hardback

For Alice and Nancy

Contents

Preface

We begin this preface by reporting the results of an experiment. On April 23, 2003, we logged onto INSPEC – the physical science and engineering online literature service – and entered the phrase "random walk." In response to this query, INSPEC delivered a list of 5010 articles, published between 1967 and that date. We then tried the plural phrase, "random walks," and were informed of 1966 more papers. Some redundancy no doubt reduces the total number of references we received to a quantity less than the sum of those two figures. Nevertheless, the point has been made. Random walkers pervade science and technology.

Why is this so? Think of a system – by which we mean just about anything – that undergoes a series of relatively small changes and that does so at random. It is more likely than not that important aspects of this system's behavior can be understood in terms of the random walk. The canonical manifestation of the random walk is Brownian motion, the jittering of a small particle as it is knocked about by the molecules in a liquid or a gas. Chitons meandering on a sandy beach in search of food leave a random walker's trail, and the bacteria *E. coli* execute a random walk as they alternate between purposeful swimming and tumbling. Go to a casino, sit at the roulette wheel and see what kind of luck you have. The height of your pile of chips will follow the rules governing a random walk, although in this case the walk is biased (see Chapter 5), in that, statistically speaking, your collection of chips will inevitably shrink.

We could go on. Random walks play a role in the analysis of the movements of stock prices. *A Random Walk down Wall Street*, by Burton Malkiel has just been published completely revised, following eight previous editions. *Random Walks, Critical Phenomena, and Triviality in Quantum Field Theory*, by Roberto Fernandez *et al*. focuses on the behavior of quantum field theory in higher dimensions. There are also *Random Walks and Other Essays*: *Ruminations of a so-so Manager*, by René Azurin; *Random Walk: A Novel for a New Age*, by Lawrence Block, and the record *Random Walks Piano Music*, by David Kraehenbuehl and Martha

Braden. Which is to say, the idea of the random walk has seeped into our collective unconscious.

In this book, we hope to acquaint the reader with powerful techniques for the analysis of random walks. The book is intended for the interested student or researcher in physics, chemistry, engineering, or mathematics. It is our hope that the level, style, and content of the book will be appealing and useful to advanced undergraduate students, graduate students, and research scientists in all disciplines. The mathematical techniques used in developing the theory are either explained in the text proper or relegated to supplements at the end of each chapter when it was thought that their inclusion would interrupt the flow of the discussion. We are hopeful that a student with a good understanding of calculus ought to be able to follow much of the analytical manipulations. However, there are instances where more advanced mathematical familiarity would be helpful.

The first five chapters of this book focus on features of a variety of unrestricted walks – that is to say, the trails left by walkers that retain no memory of where they have visited previously – including biased walks, persistent walks, continuous time walks, continuous flow walks, and walks confined to restricted regions of space. The treatment is standard for the most part. However, we attempt to introduce a language and a point of view based on generating functions, which is consistent with a more modern field-theoretical approach to the subject. This method will be fully developed in the later chapters, when we must confront the complications introduced by requiring the walk to be self-avoiding, meaning that the walker's path can never intersect itself. The generating function not only provides for a field-theoretical representation of the walker's statistical behavior, but also allows for the connection to a statistical mechanical model of magnetism. The identification of random walks and magnetism has led to a quantum jump in our understanding of the effects of self-avoidance; it makes available to the theorist the full arsenal of analytical techniques that proved so successful in unraveling the complex properties of systems that undergo continuous phase transitions.

A brief overview of the subjects covered in this book is as follows. Chapter 1 begins with a discussion of the properties of a one-dimensional walk. The chapter is intended as a sort of overture, in that points of view and tricks are introduced that we develop more fully in later chapters. Chapter 2 contains a serious discussion of the meaning, nature, and implementation of the generating function in the context of the random walk. In Chapter 3, we utilize the generating function to investigate various aspects of unrestricted walks, including recurrence, mean number of sites visited, and first passage times. Chapter 4 – which relies heavily on the wonderful little book *Random Walks in Biology*, by Berg, and contains discussions of the effects of boundary conditions on walks – introduces the electrostatic analogy for the analysis of a walk in the steady state. Biased and persistent walks make their appearance in Chapter 5. We generalize the method of treating persistent walks in one dimension to higher dimensional walks and present complete solutions for persistent walks in two and three spatial dimensions. Chapter 6 is devoted entirely to the problem of characterizing the average shape of the trail left by a random walker. We focus on a particular quantitative measure of the shape of an object that is unusually well suited to the kind of analytical tools that now exist for the characterization of the properties of a random walk.

It should be mentioned that, in each of these chapters, we attempt to point out the usefulness of the concepts of models of actual physical and biological processes as the subject is developed. No attempt is made at a comprehensive comparison between predictions of the model and experiments on particular systems. We direct the reader to Weiss' book *Aspects and Applications of the Random Walk* for such detailed comparisons.

The random walk is one of the most important and intuitively appealing examples of a statistical field theory. It is a useful pedagogical model with which to introduce someone to the latest techniques of such a theory, such as Ginzburg–Landau–Wilson effective Hamiltonians, renormalization group theory, and graphical techniques. Finding and understanding the original literature, particularly when one is branching out beyond his or her field of specialty, can be a daunting task. We have tried to reorganize and synthesize the most recent advances in the subject, which in many cases are quite formidable in formulation. In so doing, we intended to make these theories of random walks accessible to those who will find the model useful but are not well versed in the mathematical techniques upon which many recent theoretical developments are based. We set out to accomplish this task in Chapters 7 through 12.

A reading of the table of contents clearly indicates what each of these chapters entails. Here we only point out a few of the features which we found to be particularly interesting. In Chapter 7 we embark on a field theory formulation of the random walk problem *à la* S.F. Edwards, by establishing a path integral expression for the generating function. Once this is accomplished, it is straightforward to generate a perturbation expansion in a quantity which measures "self-avoidance." Doing this allows for a gentle introduction to Feynman-like graphs and an exposition of the associated graphical algebraic techniques. Using rather simple scaling arguments, we clearly demonstrate the crucial role played by dimensionality in determining the behavior of the walker, a feature that is stressed throughout the book. Finally, a mean field theory of self-avoidance is identified which then permits the infinite perturbation series to be summed. The mean field generating function yields an expression for statistical properties of the walk which shows it is exactly equivalent to Flory's treatment of self-avoidance. Chapter 8 contains a brief review of general scaling notions as they apply to the random walk.

In Chapter 9, we establish the connection between the generating function and the correlation function of a fictional magnetic system, the $O(n)$ model. This is an extremely important result, for it brings to the theorist a new set of mathematical tools developed over years by statistical physicists in their study of critical phenomena, which can now be applied to the random walk problem. Critical point scaling, critical exponents, universality, effective Hamiltonians, and renormalization group theory are now at our disposal. These topics are covered in the remaining chapters.

Once the connection between magnetism and random walks has been established, mean field theory and its extensions can be studied in well-known ways. This is done in Chapters 9 and 10. The mean field result is shown to be identical to that found previously, thereby independently demonstrating the correctness of the $O(n)$ representation of random walks. Fluctuations are incorporated in a spin wave approximation, leading to a reasonable physical rendering of the condensed state of the magnetic system as it relates to the random walker. We outline the conceptual underpinnings of the renormalization group approach and present some simple realizations of the method in Chapter 11. Chapter 12 contains a full treatment of the renormalization group as it applies to self-avoiding random walks.

We have interspersed problems throughout each chapter. These are intended to be an aid in understanding the material and to provide a way for the reader to participate in the exploration of the subject. They were not designed to be excessively long or difficult. We suggest students attempt their solution as they work their way through the chapter as a way of gauging their understanding of the material. This book is intended to be a textbook, appropriate for a stand-alone course on random walks or as a supplemental text in a field in which an understanding of random walks is required. For example, this text might prove useful in a course on polymers, or one on advanced topics in statistical mechanics, or even quantum field theory. Since our purpose here is to create a textbook, we have decided not to encumber the presentation with a plethora of footnotes and an associated comprehensive bibliography. It is our hope that the references we have included can be used to track down the original articles dealing with the various aspects of the book. We apologize to all those researchers who have made major contributions to the field and whose work is not cited herein.

This book took shape over several years, and the authors have benefited from the contributions of a number of people. We would like to express our gratitude to Professor Fereydoon Family, who stimulated our initial interest in the subject of random walks, and to Arezki Beldjenna whose contributions to the joint research that underlies much of our chapter on shapes were especially important. We are grateful to the students who sat in on the graduate seminar on random walks at

UCLA for their enthusiasm and useful comments. Special thanks go to Maria R. D'Orsogna for her careful reading of the notes that eventually became the text of this book. The problem of the shape of a random walk was brought to our attention by Professor Vladimir Privman, and for this we extend our heartfelt thanks.

The possibility of our writing a book on random walks was initially raised by Professor Lui Lam. Our decision to publish with Cambridge University Press arose from discussions with Rufus Neal. We thank him for brokering what has turned out to be an enjoyable relationship with CUP, and for introducing us to Simon Capelin, who has proven to be everything we could want in an editor. We thank Fiona Chapman for her careful, and most cheerful, efforts as copy editor. We are also grateful to Professor Warren Esty for permission to reproduce the images used in Figures 1.1 and 1.2.

Finally, we are especially indebted to Professor Peter Young, who carefully read the next-to-final version of this manuscript. His queries, comments, and suggestions resulted in a greatly improved final version.

One of the authors (GG) expresses his appreciation to Tara and Bami Das for making the early years among the best. He is also indebted to Nancy for her loving support from the beginning to the end of this project. The other author (JR) thanks his wife Alice for support, love, advice, and forbearance.

1

Introduction to techniques

This entire book is, in one way or another, devoted to a single process: the random walk. As we will see, the rules that control the random walk are simple, even when we add elaborations that turn out to have considerable significance. However, as often occurs in mathematics and the physical sciences, the consequences of simple rules are far from elementary. We will also discover that random walks, as interesting as they are in themselves, provide a basis for the understanding of a wide range of phenomena. This is true in part because random walk processes are relevant to so many processes in such a wide range of contexts. It also follows from the fact that the solution of the random walk problem requires the use of so many of the mathematical techniques that have been developed and applied in contemporary twentieth-century physics. We'll start out simply, but it won't be long before we enounter aspects to the problem that invite – indeed require – intense scrutiny.

We begin our investigations by looking at the random walk in its most elementary manifestation. The reader may find that most of what follows in this chapter is familiar material. It is, nevertheless, useful to read through it. For one thing, review is always helpful. More importantly, connections that are hinted at in the early portions of this book will play an important role in later discussion.

1.1 The simplest walk

In the simplest example of a random walk the walker is confined to a straight line. This kind of walk is called, appropriately enough, a one-dimensional walk. In this case, steps take the walker in one direction or the other. We will call those two directions "right" and "left." This makes everything easy, as we can now describe the location of the walker by drawing a horizontal line on the page and showing where on the line the walker happens to be. Let's imagine that the walker decides where its next step takes it by flipping a coin. If the coin falls heads up the walker takes a step to the right; if the coin falls tails up the walker takes a step to the left.

The outcome of a flip of the coin is equally likely to be heads or tails, so the walk is clearly unbiased, in that there is no preference for progress to the left or the right.

Suppose the walker has taken N steps. It will have flipped the coin N times. If there were n heads and $N - n$ tails, the walker will have taken n steps to the right and $N - n$ steps to the left. Suppose that each step is l meters long. Then the walker will have moved a distance

$$\begin{aligned} d &= nl - (N - n)l \\ &= l(2n - N) \end{aligned} \tag{1.1}$$

to the right. The walker will thus end up Nl meters to the left of where it started, Nl meters to the right, or somewhere in between.

Before proceeding with the analysis of the behavior of the one-dimensional walker, it is useful to inquire as to the relevance of the notion of such a walker to the real world. As it turns out, the one-dimensional walk models a number of interesting physical and mathematical processes. There is, for example, the diffusive spreading, in one dimension, of a group of molecules or small particles as the result of thermal motion. The one-dimensional walk also represents an idealization of a chain-like polymer whose monomeric units can take on one of two possible conformations. The outcome of a simple game of chance – for instance, one governed by the flip of a coin – can also be described in terms of the eventual location of a one-dimensional random walker. In this last context, one of the first applications of notions eventually associated with the random walk is due to the mathematician de Moivre in the solution of the "gambler's ruin" problem (Montroll and Shlesinger, 1983).

An immediate and fairly obvious question about the walker is the sort one generally asks about the outcome of a random process, and that is with what probability the walker ends up at a given location. That question is equivalent to asking with what probability the walker throws a certain number of heads and tails in N tosses of the coin. Another way to visualize this problem is to consider the act of flipping a coin a "trial" and to call all flips that lead to heads a success. Then, clearly, the above probability is the same as the probability of obtaining n successes in N trials. Note that this interpretation applies to trials with more than two outcomes.

Back to the random walker. Suppose we want to know the probability that the walker has gone a distance d to the right of its original position. In terms of the net distance traveled, $d = l(2n - N)$, the number of heads that were thrown is given by

$$n = \frac{1}{2}\left(\frac{d}{l} + N\right) \tag{1.2}$$

Fig. 1.1. A particular outcome of three flips of a Roman coin displaying an image of Emperor Septimius Severus (AD 193–211). Shown, left to right, is a head, then a tail, then a head.

and the number of tails is

$$N - n = \frac{1}{2}\left(N - \frac{d}{l}\right) \tag{1.3}$$

Now, the probability of throwing a specific sequence that consists of n heads and $N - n$ tails in N coin tosses is equal to $(1/2)^N$. See Figure 1.1. We arrive at the result $(1/2)^N$ for this probability by noting that the probability of either result is one half. Specifying the exact sequence of heads and tails is the same as specifying the sequence of outcomes in a set of N trials, each of which has two possible results. To obtain the probability of this sequence of outcomes, we multiply together the probabilities of each outcome in the sequence. We obtain the probability in this way because each toss of the coin is statistically independent of all other coin flips. That is, the probability of a given flip yielding a head is 1/2, regardless of how all previous tosses turned out.

The probability of throwing n heads and $N - n$ tails in *any* order is $(1/2)^N$ multiplied by the number of sequences of n heads and $N - n$ tails. See, for example, Figure 1.2. This number is simply the binomial coefficient:

$$\binom{N}{n} = \frac{N!}{n!(N-n)!}. \tag{1.4}$$

To derive the combinatorial factor in (1.4) in the case of the coin flips depicted in Figures 1.1 and 1.2, imagine the sequence of flips in Figure 1.1 as an array of coins. Then shuffle the coins in all possible ways. There are $3 \times 2 \times 1 = 3!$ ways of doing this (three possibilities for the leftmost coin, two for the next in line and only one left to place at the far right). However, in shuffling the coins, you have overcounted the number of ways in which heads and tails can turn out. Switching the first and third coins in Figure 1.1 does not change the sequence of heads and tails as both are heads. To compensate for this overcounting, we divide 3! by 2!, the number of ways of shuffling, or permuting, the two heads. This leaves us with three

Fig. 1.2. All outcomes of three flips of the Roman coin in Figure 1.1 in which one of the flips turns up tails and the other two turn up heads.

distinct ways of having two heads and a tail turning up. In general, one computes the number ways in which one can end up with n heads and $N - n$ tails in N flips of a coin by imagining the results of the flip being lined up as in Figure 1.1. Then one shuffles the coins in all possible ways, leading to the factor $N!$, which one divides by the number of ways of shuffling the n heads among themselves and the number of ways of shuffling the $N - n$ tails among themselves (Boas, 1983).

The factor in (1.4) is clearly the one that accounts for all distinct walks. It is not hard to see that the combinatorial factor $N!/n!(N - n)!$ is also equal to the number of different ways that the walker can take n steps to the right and $N - n$ steps to the left. Put another way, the factor $N!/n!(N - n)!$ *is equal to the number of walks that consist of* n *steps to the right and* $N - n$ *steps to the left.*

All this leads to the result that the likelihood that the one-dimensional walker will take n steps to the right and $N - n$ steps to the left is

$$\frac{1}{2^N}\frac{N!}{n!(N-n)!} \tag{1.5}$$

Exercise 1.1

How does the result (1.5) change when the coin is "biased" and the probability of a heads at each toss is $p \neq 1/2$? Assume that p does not change from one coin toss to the next.

We can recast our expressions in terms of the location of the walker. Using (1.2) and (1.3), we have for the number of N-step walks that take the walker a distance

d to the right of its original location

$$C(N,d) = N! \Big/ \left(\frac{N+d/l}{2}\right)! \left(\frac{N-d/l}{2}\right)! \tag{1.6}$$

and for the probability that the walker ends up a distance d to the right of its starting point

$$\begin{aligned} P(N,d) &= \frac{1}{2^N} C(N,d) \\ &= \frac{1}{2^N} N! \Big/ \left(\frac{N+d/l}{2}\right)! \left(\frac{N-d/l}{2}\right)! \end{aligned} \tag{1.7}$$

The quantity $P(N,d)$ in (1.7) is called the binomial probability distribution.

The results above allow one to calculate a good deal about the one-dimensional random walk. However, there is much that can be found out without direct recourse to them. In the next few sections we will see how much information can be extracted from fairly simple and general arguments.

1.2 Some very elementary calculations on the simplest walk

The first question that we will answer about the walker is where, on the average, it ends up. Now, the answer to that question is one that you can come up with without having to do an actual calculation. On the average, the walker will take as many steps to the right as it does to the left. The mean distance to the right from the point of departure is equal to zero.

We can do a little better than the above argument. We imagine an ensemble of walkers, performing their walks in lockstep. We note the location of each of them, and we calculate the average position by adding up the locations of all the walkers and dividing by the number of walkers in the ensemble. If the position of the ith walker is x_i, then the mean position of a set of M walkers is

$$\overline{x} = \frac{1}{M} \sum_{i=1}^{M} x_i \tag{1.8}$$

If we denote by $w(x)$ the number of walkers who have ended up at x, then $\overline{x}$ as given by the above equation is also equal to

$$\overline{x} = \frac{1}{M} \sum_{x} x w(x) \tag{1.9}$$

Given that it is equally likely that a walker will take a step to the right as to the left, we know that there will be as many walkers at $-x$ as at x, at least on the average. This means that the two terms $xw(x)$ and $-xw(-x)$ will cancel each other out in the sum in (1.9).

Of course, the cancellation will not be perfect in an actual ensemble of walkers. However, if we consider an enormous number of such ensembles, and take a sort of "super" average, then such cancellation is, indeed, achieved.

This doesn't mean that a given walker inevitably ends up where it started, or even that it ends up near its starting point. To refine our picture of the random walk, let's calculate the mean square displacement from the point of departure. This quantity, x^2, is given for a particular walk by

$$x^2 = \left(\sum_{j=1}^{N} \Delta_j\right)^2 \tag{1.10}$$

Here, Δ_j is the displacement at the jth step.[1] That is to say that at the jth step the walker moves a distance Δ_j to the right. Using

$$x = \sum_{j=1}^{N} \Delta_j \tag{1.11}$$

one can argue that $\overline{x} = 0$ by pointing out that $\overline{\Delta_j} = 0$. This is an alternative derivation of the result immediately above. In the case of $\overline{x^2}$, we expand the right hand side of (1.10) and then average.

$$\begin{aligned}
\overline{x^2} &= \overline{\left(\sum_{j=1}^{N} \Delta_j\right)^2} \\
&= \sum_j \overline{\Delta_j^2} + \sum_{j \neq k} \overline{\Delta_j \Delta_k} \\
&= \sum_j \overline{\Delta_j^2} + \sum_{j \neq k} \overline{\Delta_j} \times \overline{\Delta_k}
\end{aligned} \tag{1.12}$$

The last line in Equation (1.12) expresses the fact that each decision to take a step to the right or left is independent of every other decision. Because $\overline{\Delta_j} = 0$ for all Δ_j, the contribution of the cross terms is equal to zero. We are left with $\sum_j \overline{\Delta_j^2}$. We suppose that the length of each step is the same, so the square of the displacement at each step is equal to a fixed number, which we will call l. This means that

$$\overline{x^2} = Nl^2. \tag{1.13}$$

The root mean square displacement, which measures how far away from its starting point the walker has gotten, on the average, is, then given by

$$\sqrt{\overline{x^2}} = l\sqrt{N} \tag{1.14}$$

[1] If the walker takes a step to the left, then Δ_j is negative

The distance that the one-dimensional random walker has wandered away from its starting point goes as the square root of the number of steps it has taken.

Note that (1.14) implies that the net displacement of a random walker from the origin scales as a fractional power of the number of steps that the walker has taken. We will see that power laws pervade any quantitative discussion of the average behavior of a random walker.

Worked-out example

Generate a formula for $\overline{x^n}$ for arbitrary values of n.

Solution

The quantities on the left hand sides of (1.8) – (1.14) are known as **moments** of the random walk distribution. The quantity $\overline{x^n}$ is referred to as the nth moment of the distribution. The general form of this quantity is

$$\overline{x^n} = \frac{1}{2^N} \sum_{m=0}^{N} ((2m - N)\, l)^n \, \frac{N!}{m!(N-m)!} \tag{1.15}$$

Here, we have made use of (1.1) and (1.5). Suppose we were interested in one of the higher moments of the distribution. For example, suppose we wanted to find x^4. How would we go about doing that? We might expand the sum of the Δ_i's, raised to the fourth power, in a version of the calculation indicated in (1.12). This would lead, in due course, to an answer. In fact, calculations of $\overline{x^3}$ and $\overline{x^4}$ using (1.11) are posed as a problem later on in this chapter. However, there is another approach, based on the notion of a *generating function* (Wilf, 1994), that yields a straightforward algorithm for obtaining all moments of the distribution. What we do is note that the quantity $N!/m!(N-m)!$ is a binomial coefficient. That is, this quantity appears as the coefficient of the term w^m in the expansion of $(1+w)^N$ in powers of w:

$$(1+w)^N = \sum_{m=0}^{N} \frac{N!}{m!(N-m)!} w^m \tag{1.16}$$

Replace w by e^y, and divide by 2^N. We have

$$\frac{1}{2^N} \left(1 + \mathrm{e}^y\right)^N = \frac{1}{2^N} \sum_{m=0}^{N} \frac{N!}{m!(N-m)!} \mathrm{e}^{my} \tag{1.17}$$

Let's call the function on the left hand side of (1.17) $g(y)$. Suppose we set $y = 0$ in (1.17). We generate the equality $g(0) = (1/2^N) \sum_{m=0}^{N} N!/m!(N-m)! = (1+1)^N/2^N = 1$.

To find the moments, we take derivatives. For example,

$$\begin{aligned}\left.\frac{\mathrm{d}}{\mathrm{d}y}g(y)\right|_{y=0} &= \left.\frac{1}{2^N}\sum_{m=0}^{N}\frac{N!}{m!(N-m)!}m\mathrm{e}^{my}\right|_{y=0}\\ &= \frac{1}{2^N}\sum_{m=0}^{N}\frac{N!}{m!(N-m)!}m\\ &\equiv \overline{m}\\ &= \left.\frac{\mathrm{d}}{\mathrm{d}y}\frac{1}{2^N}(1+\mathrm{e}^y)^N\right|_{y=0}\\ &= \left.N\mathrm{e}^y\frac{(1+\mathrm{e}^y)^{N-1}}{2^N}\right|_{y=0}\\ &= N\frac{(1+1)^{N-1}}{2^N}\\ &= \frac{N}{2}\end{aligned} \tag{1.18}$$

This tells us both that $\overline{m} = N/2$ and that $\overline{m} = \mathrm{d}g(y)/\mathrm{d}y|_{y=0}$. We can readily generalize this result to

$$\overline{m^n} = \left.\frac{\mathrm{d}^n}{\mathrm{d}y^n}g(y)\right|_{y=0} \tag{1.19}$$

Making use of this result – and noting that $x = N - 2m$ – we can rewrite the expression for x^n as follows:

$$x^n = l^n\left(N - 2\frac{\mathrm{d}}{\mathrm{d}y}\right)^n g(y)\Bigg|_{y=0} \tag{1.20}$$

We can do a bit more. We rewrite the function $g(y)$ as follows:

$$\begin{aligned}g(y) &= \mathrm{e}^{Ny/2}\left(\frac{\mathrm{e}^{y/2}+\mathrm{e}^{-y/2}}{2}\right)^N\\ &= \mathrm{e}^{Ny/2}\cosh(y/2)^N\end{aligned} \tag{1.21}$$

Then, we note that

$$\begin{aligned}&\left(N - 2\frac{\mathrm{d}}{\mathrm{d}y}\right)\mathrm{e}^{Ny/2}\cosh(y/2)^N\\ &= \cosh(y/2)^N\left(N - 2\frac{\mathrm{d}}{\mathrm{d}y}\right)\mathrm{e}^{Ny/2} - 2\frac{\mathrm{d}}{\mathrm{d}y}\cosh(y/2)^N\\ &= 0 - 2\frac{\mathrm{d}}{\mathrm{d}y}\cosh(y/2)^N\end{aligned} \tag{1.22}$$

We can carry this calculation out for the case of higher powers of $N - 2\mathrm{d}/\mathrm{d}y$ as applied to the function $g(y)$, and we find in general that

$$\left(N - 2\frac{\mathrm{d}}{\mathrm{d}y}\right)^n g(y) = (-2)^n \frac{\mathrm{d}^n}{\mathrm{d}y^n} \cosh(y/2)^N \tag{1.23}$$

Exercise 1.2
Prove (1.23) by induction, or any other method you like.

This means that

$$\overline{x^n} = (-2l)^n \frac{\mathrm{d}^n}{\mathrm{d}y^n} \cosh(y/2)^N \bigg|_{y=0} \tag{1.24}$$

Then,

$$\begin{aligned}
\overline{x^2} &= 4l^2 \frac{\mathrm{d}^2}{\mathrm{d}y^2} \cosh(y/2)^N \bigg|_{y=0} \\
&= 4\left(\frac{N\cosh(y/2)^N}{4} + \frac{(-1+N)N\cosh(y/2)^{-2+N}\sinh(y/2)^2}{4}\right)\bigg|_{y=0} \\
&= Nl^2
\end{aligned} \tag{1.25}$$

as found earlier (see (1.13)).

The next non-zero moment is $\overline{x^4}$. We find

$$\begin{aligned}
\overline{x^4} &= 16l^4 \frac{\mathrm{d}^4}{\mathrm{d}y^4} \cosh(y/2)^N \bigg|_{y=0} \\
&= \frac{l^4}{8} N \cosh\left(\frac{y}{2}\right)^{-4+N} \big((-4+N)(8+3(-4+N)N) \\
&\qquad - 4(-4+(-4+N)(-2+N)N)\cosh(y) + N^3 \cosh(2y)\big)\big|_{y=0} \\
&= l^4 N(-2+3N)
\end{aligned} \tag{1.26}$$

Note that the average of the fourth power of the distance of a one-dimensional random walker from its point of origin has a term going as the square of the number of steps, N, and also a term going linearly in N. At large values of N, the term going as N^2 dominates the expression. Comparing (1.26) and (1.25), we see that when N is very large

$$\overline{x^4}/(\overline{x^2})^2 \approx 3 \tag{1.27}$$

Exercise 1.3

Use the relationship $x = \sum_{j=1}^{N} \Delta_j$ for a one-dimensional walk – where Δ_j is the displacement to the right of the walker at the ith step – to find $\overline{x^3}$ and $\overline{x^4}$. Make use of the fact that $\overline{\Delta_i^n}$ is equal to zero when n is odd and also that $\overline{\Delta_i^n} = l^n$ when n is even. You will also make use of the fact that $\overline{\Delta_{j_1}^{n_1} \Delta_{j_2}^{n_2} \cdots \Delta_{j_m}^{n_m}} = \overline{\Delta_{j_1}^{n_1}} \times \overline{\Delta_{j_2}^{n_2}} \times \cdots \times \overline{\Delta_{j_m}^{n_m}}$ when $j_1 \neq j_2 \neq \cdots \neq j_m$.

1.3 Back to the probability distribution

Let's return to the combinatorial factor in (1.4). Although the expression is complete, in that we know perfectly well how to calculate each term in it, it is not of immediate analytical use, especially when N, the number of random walk steps, is large. We will now remedy this shortcoming by making use of Stirling's formula for the factorial to produce an expression more amenable to calculation. Stirling's formula is

$$\ln n! \approx n \ln\left(\frac{n}{\mathrm{e}}\right) + \frac{1}{2}\ln(2\pi n) \tag{1.28}$$

An approximation that holds with greater accuracy as n is increased.

1.3.1 Derivation of Stirling's formula

The approximate form that we will use follows from the well-known expression for the gamma function

$$\Gamma(x) = \int_0^\infty w^{x-1} \mathrm{e}^{-w}\, \mathrm{d}w \tag{1.29}$$

The relationship between the gamma function and the factorial is

$$N! = \Gamma(N+1) \tag{1.30}$$

This means

$$N! = \int_0^\infty w^N \mathrm{e}^{-w}\, \mathrm{d}w \tag{1.31}$$

The proof of the equality is readily established by integration by parts.

Figure 1.3 is a plot of the integrand in (1.31) when $N = 10$. Superimposed on that plot is a Gaussian, shown as a dashed curve, which will be used to approximate the integrand in the derivation of Stirling's formula. How do we arrive at the approximation by a Gaussian? First, we notice that the integrand is maximized

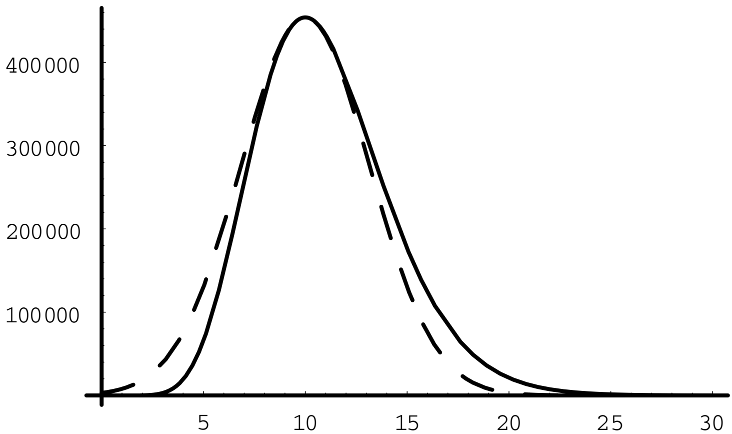

Fig. 1.3. The integrand $w^N e^{-w}$, in (1.31), when $N = 10$, along with the Gaussian curve, shown dashed here, which will be used to approximate that integrand, in the derivation of Stirling's formula.

with $w = N$. We notice this by replacing w in the integrand by $N + \delta$, and then by exponentiating everything in the integrand. This exponentiation yields

$$N! = \int_{-N}^{\infty} dw \exp\left[N \ln(N + \delta) - N - \delta\right] \tag{1.32}$$

Focusing on the exponent and expanding in powers of δ:

$$\begin{aligned} N \ln(N + \delta) - (N + \delta) &= N \ln N + N \ln(1 + \delta/N) - N - \delta \\ &= (N \ln N - N) + N \left(\frac{\delta}{N} - \frac{1}{2}\frac{\delta^2}{N^2} + \cdots \right) - \delta \\ &= (N \ln N - N) - \frac{\delta^2}{2N} + O\left(\delta^3\right) \\ &\equiv (N \ln N - N) - \frac{(w - N)^2}{2N} + \cdots \end{aligned} \tag{1.33}$$

The Gaussian curve in Figure 1.3 is the function $\exp[10 \ln 10 - 10 - (w - 10)^2/20]$. Suppose we replace the integrand by that Gaussian approximation. We then get the following result for the integration, leading to the factorial

$$N! \approx \sqrt{2\pi N} \exp\left[N(\ln N - N)\right] \tag{1.34}$$

To see how good an approximation it is, let's compare the natural logarithm of 10! with the natural logarithm of the right hand side of (1.34).

$$\ln 10! = 15.1044 \tag{1.35}$$

$$\ln\left(\sqrt{2\pi N} \exp\left[N(\ln N - N)\right]\right) = 15.0961 \tag{1.36}$$

The fractional difference between the right hand side of (1.35) and the right hand side of (1.36) is about five parts in 10^4. The approximation gets even better as N increases. When $N = 100$, the fractional difference between the logarithm of Stirling's formula and the log of the exact factorial is two parts in 10^6.

The formula works if n is large compared to 1. This means that the combinatorial factor in (1.4) is well-approximated by

$$\exp\left[N\ln\left(\frac{N}{\mathrm{e}}\right)+\frac{1}{2}\ln(2\pi N)-n\ln\left(\frac{n}{\mathrm{e}}\right)+\frac{1}{2}\ln(2\pi n)\right.$$
$$\left.-(N-n)\ln\left(\frac{N-n}{\mathrm{e}}\right)+\frac{1}{2}\ln(2\pi(N-n))\right] \tag{1.37}$$

Let $n = \frac{N}{2} + m$ with $m \ll N$. Then the exponent in (1.37) can be expanded as follows. We start with

$$\ln\left(\frac{N}{2}+m\right)=\ln\left(\frac{N}{2}\right)+\frac{2m}{N}+\frac{1}{2}\left(\frac{2m}{N}\right)^2+\cdots \tag{1.38}$$

With the use of this equation, one obtains

$$N\ln 2-\frac{n^2}{2N}-\frac{1}{2}\ln 2\pi N+O\left(\frac{n^3}{N^2},\frac{n}{N}\right) \tag{1.39}$$

so the combinatorial factor has the form

$$\frac{2^N}{\sqrt{2\pi N}}\exp\left[-\frac{n^2}{2N}+O\left(\frac{n^3}{N^2},\frac{n}{N}\right)\right] \tag{1.40}$$

The number m is equal to $n - N/2$, and since by (1.2) $n = d/2l + N/2$, we have $m = d/2l$. This means that the likelihood that a walker will end up a distance d from its point of departure is given by

$$\frac{1}{\sqrt{2\pi N}}\exp\left(-\frac{d^2}{2Nl^2}\right). \tag{1.41}$$

In arriving at (1.41), we have divided by the requisite factor of 2^N to arrive at a probability density that is normalized to one.

The expression in (1.41) is a Gaussian. We will encounter this ubiquitous form repeatedly in the course of our investigation of random walk statistics. It reflects the consequences of the central limit theorem of statistics (Feller, 1968), as it applies to the random walk process.

Exercise 1.4

If N is large, then we can approximate the derivative of the log of $N!$ as follows:

$$\frac{d}{dN} \ln N! \approx \frac{\ln N! - \ln(N-1)!}{N-(N-1)}$$

Use this approximation to derive the leading contribution to Stirling's formula for $N!$ (the first term on the right hand side of (1.28)).

1.4 Recursion relation for the one-dimensional walk

There is another way to investigate the one-dimensional random walk. The number of N-step walks that begin at a given location and end up at another one can be related to the number of $N-1$-step walks that start at the same location and end up nearby. If $C(N; x, y)$ is equal to the number of walks that start at x and end up at y then

$$C(N; x, y) = C(N-1; x, y-l) + C(N-1; x, y+l) \tag{1.42}$$

The formula (1.42) states mathematically that the number of N-step walks starting at x and ending at y is equal to the sum of the number of $N-1$-step walks that start at x and end up at all points adjacent to y. This statement reflects the fact that the last step that a walker takes before ending up at the point y is from a neighboring location. This fact tells us that the sequence of steps taken by our walker, considered as a sequence of random events has the form of a *Markovian* process of the first order (Boas, 1983; Feller, 1968). That is, the probability of occurrence of a given event is independent of the history consisting of all previous events. In future chapters we will encounter higher order Markovian chains, and even some that are non-Markovian.

The recursion relation (1.42) can be utilized to derive a familiar formula for the combinatorial factors. Recall (1.4). This expression is for the number of N-step walks that consist of n steps to the right and $N-n$ steps to the left. Replacing the terms in (1.42) by the equivalent expressions in terms of the combinatorial factors, we have

$$\frac{N!}{n!(N-n)!} = \frac{(N-1)!}{(n-1)!(N-n)!} + \frac{(N-1)!}{n!(N-n-1)!} \tag{1.43}$$

That (1.43) is true can be readily verified. It is also the relation between combinatorial factors that leads to Pascal's triangle.

There is more that can be done with this recursion relation. If one assumes a gentle dependence on the end point y – which is, in fact, the case when N is large – the recursion relation can be approximated by a differential equation. This is accomplished by rewriting (1.42) as follows:

$$\begin{aligned} C(N+1;x,y) &= (C(N;x,y-l) + C(N;x,y+l) - 2C(N;x,y)) \\ &\quad + 2C(N;x,y) \\ &= l^2 \left(\frac{C(N;x,y-l) + C(N;x,y+l) - 2C(N;x,y)}{l^2} \right) \\ &\quad + 2C(N;x,y) \\ &\approx l^2 \frac{\partial^2 C(N;x,y)}{\partial y^2} + 2C(N;x,y) \end{aligned} \tag{1.44}$$

Another way to write this equation is

$$C(N+1;x,y) - 2C(N;x,y) = l^2 \frac{\partial^2 C(N;x,y)}{\partial y^2} \tag{1.45}$$

Suppose we replace $C(N;x,y)$ by $2^N P(N;x,y)$, where $P(N;x,y)$ is the probability that a walker starting out at y ends up at x after N steps. Equation (1.45) becomes

$$P(N+1,x,y) - P(N;x,y) = \frac{l^2}{2} \frac{\partial^2 P(N;x,y)}{\partial y^2} \tag{1.46}$$

Again, imagine that N is large and that $P(N;x,y)$ is a slowly varying function of N. Then, we approximate the right hand side of (1.46) by $\partial P(N;x,y)/\partial N$, and we are left with the equation

$$\frac{\partial P(N;x,y)}{\partial N} = \frac{l^2}{2} \frac{\partial^2 P(N;x,y)}{\partial y^2} \tag{1.47}$$

This equation occupies a place of central importance, not only in the study of the random walk, but also in physical and biological sciences, as well as in engineering. It is the diffusion equation. While there are a variety of ways in which it can be solved, we will write down a solution with the understanding that one can verify that it works. We assume that the reader has encountered the equation and its solution previously, and assert that it is

$$P(N;x,y) = \frac{\alpha}{\sqrt{N}} \exp\left(\frac{(x-y)^2}{2l^2 N} \right) \tag{1.48}$$

Exercise 1.5
Verify (1.48) by direct substitution into (1.47).

1.5 Backing into the generating function for a random walk

So far our analysis of the statistics of the one-dimensional random walk problem is the standard introduction to the subject that one finds in any elementary exposition of the process. In the remaining portion of the section we would like to play some games with the solution that we derived in (1.6) as a gentle way of initiating the reader to the more advanced analytical techniques presented in subsequent sections. It may seem at first that the development represents a retreat from the results obtained earlier on, in that the solution is, in a sense, "hidden" in the expressions to be derived. However, what we will have at the end is a set of definitions and relationships that can be generalized into a powerful approach to the properties of more generally defined random walks.

Recall that the expression on the right hand side of that equation is the combinatorial factor in (1.4), with n, the number of steps to the right, expressed in terms of d through (1.2). The factor $N!/n!(N-n)!$ also appears in the expansion of the expression $(1+w)^N$ in powers of w. That is

$$(1+w)^N = \sum_{n=0}^{N} \frac{N!}{n!(N-n)!} w^n \tag{1.49}$$

It is a straightforward exercise to verify that the right hand side of (1.6) is the coefficient of $\mathrm{e}^{\mathrm{i}qd}$ in

$$\left(\mathrm{e}^{\mathrm{i}ql} + \mathrm{e}^{-\mathrm{i}ql}\right)^N \equiv \chi(q)^N \tag{1.50}$$

The above means that the number of N-step walks that take the walker a distance d to the right of its starting point is the coefficient of $\mathrm{e}^{\mathrm{i}qd}$ in the expansion in terms of $\mathrm{e}^{\mathrm{i}q}$ of the expression $(2\cos q)^N$. There is a simple way to obtain that term. One merely performs the integral

$$\frac{l}{2\pi} \int_{-\pi/l}^{\pi/l} \mathrm{e}^{-\mathrm{i}qd} \chi(q)^N \, \mathrm{d}q \tag{1.51}$$

In other words, the number of walks of interest is obtained by taking the inverse Fourier transform of $\chi(q)$ raised to the Nth power. How (1.51) comes about is more fully explained in the next section.

It is possible to regain the Gaussian form for the number of N-step walks by performing the integral above, with the use of a couple of tricks and approximations. First, we rewrite the expression for $\chi(q)$ as follows.

$$\begin{aligned}
\chi(q) &= 2\cos ql \\
&= \mathrm{e}^{\ln(2\cos ql)} \\
&= 2\mathrm{e}^{\ln(\cos ql)} \\
&= 2\mathrm{e}^{\ln(1-q^2l^2/2+\cdots)} \\
&= 2\mathrm{e}^{-q^2l^2/2+O(q^4)}
\end{aligned} \tag{1.52}$$

If we neglect the terms of order q^4 in the exponent,

$$\chi(q)^N \approx 2^N \mathrm{e}^{-Nq^2l^2/2} \tag{1.53}$$

Plugging this result into (1.51), we obtain

$$\frac{l}{2\pi}\int_{-\pi/l}^{\pi/l} \mathrm{e}^{-\mathrm{i}qd} 2^N \mathrm{e}^{-Nq^2l^2/2}\,\mathrm{d}q \approx \frac{2^N}{\sqrt{2\pi N}}\mathrm{e}^{-d^2/2Nl^2} \tag{1.54}$$

This is the same result as is given in (1.41). The integral was evaluated by assuming that the upper and lower limits can be taken to plus and minus infinity. The error that this assumption entails can be shown to be negligible.

There is more. Suppose we perform the geometrical sum

$$g(z,q) = \sum_{N=0}^{\infty} \chi(q)^N z^N = \frac{1}{1 - z\chi(q)} \tag{1.55}$$

The quantity $\chi(q)^N$, entering into (1.51), is the coefficient of z^N in the expansion of the right hand side of (1.55) in powers of the quantity z. The functions defined by expansions of the kind given in (1.55) are called *generating functions*. A large portion of this book is devoted to the exploration of their properties. If we perform a further expansion of the "structure function" $\chi(q)$ in powers of q, we have

$$\chi(q) \approx 2\mathrm{e}^{-q^2l^2/2} \approx 2\left(1 - \frac{q^2l^2}{2}\right) \tag{1.56}$$

This expansion is accurate for our purposes as long as the number of steps in the walk, N, is large and the end-to-end distance, d, is not too great. As a practical matter, we require $d \ll N$.

The right hand side of (1.55) is, then, replaced by

$$\frac{1}{1 - 2z + zq^2l^2} \tag{1.57}$$

and the number of N-step walks that displace the walker a distance d from its starting point is equal to the inverse Fourier transform of the coefficient of z^N of the expression in (1.57).

At this point, it may have seemed as if the transformations that have been performed have had the effect of complicating, rather than simplifying, the problem at hand. After all, the inverse Fourier transform is bad enough. The extraction of a coefficient in a power series can be an arbitrarily difficult procedure. In the case at hand, one has the right hand side of (1.55). As it turns out, there are also some general prescriptions and a class of tricks that ease the difficulty of the latter procedure. To find the coefficient of z^N in the function $f(z)$, one simply performs the

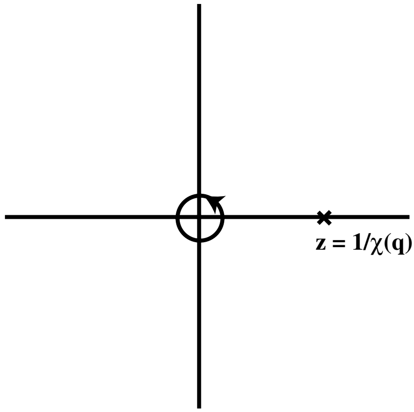

Fig. 1.4. Contour for the integral in (1.58). The pole at $z = 1/\chi(q)$ when $f(z)$ is given by (1.55) is indicated.

following contour integral

$$\frac{1}{2\pi i} \oint_c \frac{f(z)}{z^{N+1}} \, dz. \tag{1.58}$$

The contour encircles the origin, as shown in Figure 1.4. It is assumed that there is no significant singularity of the function $f(z)$ inside the closed contour. The alert reader will recognize this as Cauchy's formula (Jeffreys, 1972) for $N! d^N/dz^N \; f(z)|_{z=0}$. The evaluation of the contour integral when $f(z)$ looks like the right hand side of (1.55) is relatively straightforward. One deforms the contour so that it encloses the pole at $z = 1/\chi(k)$. Applying the formulas that apply to integration around simple poles, one recovers the appropriate coefficient.

There is another way to recover the result for the number of walks from the generating function. This method simplifies the extraction of the desired expression when the number of steps, N, is large. Let the generating function be given by the approximate form in (1.57). The integral over z is accomplished by exponentiating the generating function and the denominator z^{N+1}. The integral is now over the function

$$\exp\left[-(N+1)\ln z - \ln\left(1 - 2z + zq^2l^2\right)\right] \tag{1.59}$$

The integral is evaluated by looking for an extremum in the exponent of the expression above. The equation for the extremum is

$$-\frac{N+1}{z} + \frac{(2 - q^2l^2)}{1 - 2z + zq^2l^2} = 0 \tag{1.60}$$

Because N is large, the denominator of the second term on the left hand side of (1.60) will be small. Writing $z = 1/(2 - q^2l^2) + \delta$, we find δ of order $1/(N+1)$.