1

First-Passage Fundamentals

1.1. What Is a First-Passage Process?

This book is concerned with the first-passage properties of random walks and diffusion, and the basic consequences of first-passage phenomena. Our starting point is the *first-passage probability*; this is the probability that a diffusing particle or a random-walk *first* reaches a specified site (or set of sites) at a specified time. The importance of first-passage phenomena stems from its fundamental role in stochastic processes that are triggered by a first-passage event. Typical examples include fluorescence quenching, in which light emission by a fluorescent molecule stops when it reacts with a quencher; integrate-and-fire neurons, in which a neuron fires only when a fluctuating voltage level first reaches a specified level; and the execution of buy/sell orders when a stock price first reaches a threshold. Further illustrations are provided throughout this book.

1.1.1. A Simple Illustration

To appreciate the essential features of first-passage phenomena, we begin with a simple example. Suppose that you are a nervous investor who buys stock in a company at a price of \$100. Suppose also that this price fluctuates daily in a random multiplicative fashion. That is, at the end of each day the stock price changes by a multiplicative factor $f < 1$ or by f^{-1} compared with the previous day's price, with each possibility occurring with probability $1/2$ (Fig. 1.1). The multiplicative change ensures that the price remains positive. To be concrete, let's take $f = 90\%$ and suppose that there is a loss on the first day so that the stock price drops to \$90. Being a nervous investor, you realize that you don't have the fortitude to deal with such a loss and wish to sell your stock. However, because the price fluctuates randomly you also think that it might be reasonable to wait until the stock recovers to its initial price before selling out.

Some of the basic questions you, as an skittish investor, will likely be asking yourself are: (1) Will I eventually break even? (2) How long do I have to wait

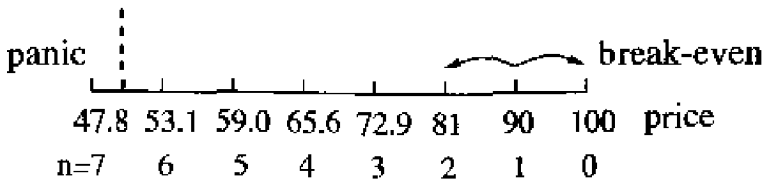


Fig. 1.1. Daily stock price, when it changes by a multiplicative factor of $f = 0.9$ or $f^{-1} = 1.11\cdots$ with equal probabilities. The starting price is \$100. Panic selling occurs if the stock price drops to less than half its initial value.

until I break even? (3) While I am waiting to break even, how low might the stock price go? (4) Is it a good idea to place a limit order, i.e., automatically sell if the stock falls below a specified price? Clearly, the answers to these questions will help you to make an informed decision about how to invest in this toy market.

To make these questions precise and then answer them, note that the price performs a symmetric random walk in n, where $n = N_+ - N_-$ is the difference in the number of "up" and "down" days, N_+ and N_-, respectively. After $N = N_+ + N_-$ trading days, the stock price will be $f^n \times \$100$. In our example, the random walk started at $n = 0$ (price \$100) and after one day it jumped to $n = 1$, corresponding to a stock price of \$90. The question of break even after a first-day loss can be rephrased as, What is the probability that a random walk that starts at $n = 1$ *eventually* returns to, or equivalently, eventually hits $n = 0$? As discussed in Section 1.5, this eventual return probability equals one; you are sure to recoup your initial loss. However, the time required for recouping this loss, averaged over *all* possible histories of the stock price, is infinite! Just as disconcerting, while you are waiting forever to ensure recovery of your initial investment, your capital can achieve a vanishingly small value. You would need a strong stomach to survive this stock market! These seemingly paradoxical features have a natural explanation in terms of the first-passage probability of a random walk. Our goal will be to develop a general understanding of first-passage properties for both random walk and diffusion phenomena in a variety of physically relevant situations.

An important aspect of first-passage phenomena is the conditions by which a random-walk process terminates. Returning to our stock market with 10% daily price fluctuations, suppose that you would panic and sell out if the stock price were to sink to less than one-half of its initial value, in addition to selling if and when the price returns to its original value. Selling out at a loss would occur the *first* time that there are 7 more down days than up days. We can then ask, What it the probability of selling at break even or selling at a loss? How long will it take before one of these two events occurs? These

are the types of questions that are answered by the study of first-passage phenomena.

1.1.2. Fundamental Issues

The basic questions of first-passage phenomena are the following:

- What is the time dependence of the first-passage probability $F(\vec{r}, t)$? This is the probability that a random walk or a diffusing particle hits a specified point $\vec{r}$ *for the first time* at time t. More generally, what is the first-passage probability for a diffusing particle to hit a *set* of points?

As we shall discuss in Section 1.2, the first-passage probability can be obtained directly from the more familiar *occupation probability* $P(\vec{r}, t)$. This is the probability that a diffusing particle is located at $\vec{r}$ at time t. Note that we are using the terms random walk and diffusing particle loosely and interchangeably. Although these two processes are very different microscopically, their long-time properties – including first-passage characteristics – are essentially the same. In Section 1.3 it is shown how diffusion is merely the continuum limit of any sufficiently well-behaved random-walk process. Thus in the rest of this book we will use the description that best suits the situation under discussion.

In many cases, the diffusing particle physically disappears or "dies" when the specified point or set of points is hit. We can therefore think of this set as an absorbing boundary for the particle. This picture then leads to several more fundamental first-passage-related questions:

- What is the survival probability $S(t)$, that is, the probability that a diffusing particle has not hit the absorbing boundary by time t?
- How long does it take for the diffusing particle to die, that is, hit the absorbing boundary? More precisely, what is the mean time until the particle hits a site on the absorbing boundary as a function of the particle's starting point? This is often referred to as the mean first-passage time or mean exit time.
- Where on the absorbing boundary does the particle get absorbed?

Another interesting feature arises in systems for which the boundary B consists of disjoint subsets, for example, $B = B_1 \cup B_2$, with B_1 and B_2 nonoverlapping. Then it is worthwhile to determine whether the diffusing particle is eventually absorbed in B_1 or in B_2 as a function of the initial particle position. This is often known as the *splitting probability*. For the nervous-investor

example presented above, the splitting probabilities refer to the probabilities of ultimately selling at break even or at a 50% loss. More precisely:

- For an absorbing boundary that can be decomposed into disjoint subsets B_1 and B_2, what is the splitting probability, namely, the probability that a diffusing particle will eventually be trapped on B_1 or trapped on B_2 as a function of the initial particle position?

We conclude this introduction with a brief synopsis of the answers to the above questions. For a diffusing particle in a finite domain with an absorbing boundary, the survival probability $S(t)$ typically decays exponentially with time (Chap. 2). Roughly speaking, this exponential decay sets in once the displacement of the diffusing particle becomes comparable with the linear size of the domain. Correspondingly, the mean time $\langle t \rangle$ until the particle hits the boundary is finite. On the other hand, if the domain is unbounded (Chaps. 3 and 5–7) or if boundaries move (Chap. 4), then the geometry of the absorbing boundary is an essential feature that determines the time dependence of the survival probability. For such situations, $S(t)$ either asymptotically approaches a nonzero value or it decays as a power law in time, with the decay exponent a function of the boundary geometry. In our nervous-investor example, the techniques of Chap. 2 will tell us that (s)he will (fortunately) break even 6/7 of the time and will be in the market for 6 days, on average, before selling out.

To determine where on the boundary a diffusing particle is absorbed, we shall develop a powerful but simple analogy between first-passage and electrostatics (Section 1.6). From this classic approach, we will learn that the probability for a particle, which starts at $\vec{r}_0$, to eventually exit at a point $\vec{r}$ on the boundary equals the electric field at $\vec{r}$, when all of the boundaries are grounded conductors and a point charge is placed at $\vec{r}_0$. From this electrostatic analogy, the splitting probability between two points is simply the ratio of the corresponding electrostatic potentials at these points. Because the potential is a linear function of the distance between the source and the observer, we can immediately deduce the splitting probabilities of 6/7 (break even) and 1/7 (panic sell at a 50% loss) of the nervous-investor example.

In the rest of this chapter, basic ideas and techniques are introduced to aid in understanding the first-passage probability and the fundamental quantities that derive from it. In the remaining chapters, many features of first-passage phenomena are illustrated for diffusion processes in a variety of physically relevant geometries and boundary conditions. Many of these topics are covered in books that are either devoted entirely to first-passage processes [Kemperman (1961), Dynkin & Yushkevich (1969), Spitzer (1976), and Syski (1992)] or

in books on stochastic processes that discuss first-passage processes as a major subtopic [Cox & Miller (1965), Feller (1968), Gardiner (1985), Risken (1988), Hughes (1995), and van Kampen (1997)].

1.2. Connection between First-Passage and Occupation Probabilities

We now discuss how to relate basic first-passage characteristics to the familiar occupation probability of the random walk or the probability distribution of diffusion. An important starting fact is that the survival probability $S(t)$ in an absorbing domain equals the integral of the first-passage probability over all time and over the spatial extent of the boundary. This is simply a consequence of the conservation of the total particle density. Thus all first-passage characteristics can be expressed in terms of the first-passage probability itself.

We now derive the relation between the first-passage probability and the probability distribution. Derivations in this spirit are given, e.g., in Montroll and Weiss (1965), Fisher (1984), and Weiss (1994). We may express this connection in equivalent ways, either in terms of discrete-space and -time or continuous-space and -time variables, and we will use the representation that is most convenient for the situation being considered. Let us start with a random walk in discrete space and time. We define $P(\vec{r}, t)$ as the occupation probability; this is the probability that a random walk is at site $\vec{r}$ at time t when it starts at the origin. Similarly, let $F(\vec{r}, t)$ be the first-passage probability, namely, the probability that the random walk visits $\vec{r}$ for the first time at time t with the same initial condition. Clearly $F(\vec{r}, t)$ asymptotically decays more rapidly in time than $P(\vec{r}, t)$ because once a random walk reaches $\vec{r}$, there can be no further contribution to $F(\vec{r}, t)$, although the same walk may still contribute to $P(\vec{r}, t)$.

Strategically, it is simplest to write $P(\vec{r}, t)$ in terms of $F(\vec{r}, t)$ and then invert this relation to find $F(\vec{r}, t)$. For a random walk to be at $\vec{r}$ at time t, the walk must first reach $\vec{r}$ at some earlier time step t' and then return to $\vec{r}$ after

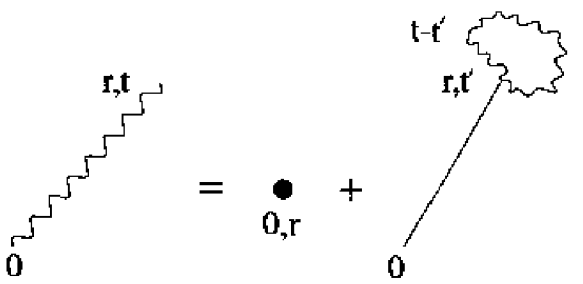


Fig. 1.2. Diagrammatic relation between the occupation probability of a random walk (propagation is represented by a wavy line) and the first-passage probability (straight line).

$t - t'$ additional steps (Fig. 1.2). This connection between $F(\vec{r}, t)$ and $P(\vec{r}, t)$ may therefore be expressed as the convolution relation

$$P(\vec{r}, t) = \delta_{\vec{r},0}\delta_{t,0} + \sum_{t' \le t} F(\vec{r}, t')\, P(0, t - t'), \tag{1.2.1}$$

where $\delta_{t,0}$ is the Kronecker delta function. This delta function term accounts for the initial condition that the walk starts at $\vec{r} = 0$. Note that returns *before* time t are also permissible as long as there is also a return $t - t'$ steps after the first return. Because of the possibility of multiple visits to $\vec{r}$ between time t' and t, the return factor involves P rather than F.

This convolution equation is most conveniently solved by introducing the generating functions,

$$P(\vec{r}, z) = \sum_{t=0}^{\infty} P(\vec{r}, t) z^t, \qquad F(\vec{r}, z) = \sum_{t=0}^{\infty} F(\vec{r}, t) z^t.$$

If we were dealing with a random walk in continuous time, we would first replace the sum over discrete time in Eq. (1.2.1) with an integral and then use the Laplace transform. However, the ensuing asymptotic results would be identical. To solve for the first-passage probability, we multiply Eq. (1.2.1) by z^t and sum over all t. We thereby find that the generating functions are related by

$$P(\vec{r}, z) = \delta_{\vec{r},0} + F(\vec{r}, z) P(0, z). \tag{1.2.2}$$

Thus we obtain the fundamental connection

$$F(\vec{r}, z) = \begin{cases} \dfrac{P(\vec{r}, z)}{P(0, z)}, & \vec{r} \neq 0 \\ 1 - \dfrac{1}{P(0, z)}, & \vec{r} = 0 \end{cases}, \tag{1.2.3}$$

in which the generating function, or equivalently, the Laplace transform of the first-passage probability, is determined by the corresponding transform of the probability distribution of diffusion $P(\vec{r}, t)$. This basic relation and its many consequences are also treated extensively in Montroll (1965), Montroll and Weiss (1965), Weiss and Rubin (1983), and Weiss (1994).

Because this probability distribution is basic to understanding diffusion and because it also determines the first-passage probability, several complementary approaches are presented to derive the first-passage probability in Section 1.3. In Section 1.4, it is shown how to relate basic probabilities in real time with their corresponding generating function or Laplace transform. Armed with this information, we then obtain the asymptotics of the first-passage probability in Section 1.5.

1.3. Probability Distribution of a One-Dimensional Random Walk

We now discuss basic features of the probability distribution of a random walk, as well as the relation between random walks and diffusion. Much of this discussion is standard but is included for completeness and to illustrate the universal asymptotic behavior of the various representations of random walks in terms of diffusion. Derivations of varying degrees of completeness and sophistication can be found, e.g., in Reif (1965) and van Kampen (1997). In deriving $P(\vec{r}, t)$, we treat in detail the nearest-neighbor random walk in one dimension and merely quote results for higher dimension as needed. We start with the easily visualized discrete-space and -time hopping process and then proceed to the continuum diffusion limit. The order of presentation is chosen to help advertise the relative simplicity of the continuum representation. These derivations also serve to introduce the mathematical tools that will be used in treating first-passage properties, such as Fourier and Laplace transforms, the generating function, and basic asymptotic analysis.

1.3.1. Discrete Space and Time

Consider a particle that hops at discrete times between neighboring sites on a one-dimensional chain with unit spacing. Let $P(x, N)$ be the probability that the particle is at site x at the Nth time step. The evolution of this occupation probability is described by the master equation

$$P(x, N+1) = pP(x-1, N) + qP(x+1, N). \tag{1.3.1}$$

This states that the probability for the particle to be at x at time $N+1$ is simply p times the probability of being at $x-1$ at time N (contribution of a step to the right) plus q time the probability of being at $x+1$ at time N (step to the left). The case $p = q = \frac{1}{2}$ is the symmetric random walk, whereas for $p > q$ there is a uniform bias to the right and for $p < q$ a bias to the left (see Fig. 1.3).

Because of translational invariance in both space and time, it is natural to solve this equation by transform techniques. For this example, we therefore

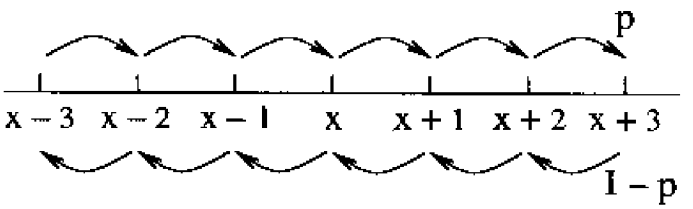


Fig. 1.3. The hopping processes for the one-dimensional nearest-neighbor random walk defined by Eq. (1.3.1).

define the combined generating function and Fourier transform:

$$P(k, z) = \sum_{N=0}^{\infty} z^N \sum_{x=-\infty}^{\infty} e^{ikx} P(x, N).$$

In all the discussions that follow, either the arguments of a function or the context (when obvious) will be used to distinguish the transform from the function itself.

Applying this combined transform to the master equation, and multiplying by one additional factor of z, gives

$$\sum_{N=0}^{\infty} \sum_{x=-\infty}^{\infty} z^{N+1} e^{ikx} \left[P(x, N+1) = pP(x-1, N) + qP(x+1, N)\right]. \tag{1.3.2}$$

The left-hand side is just the generating function $P(k, z)$, except that the term $P(x, N = 0)$ is missing. Similarly, on the right-hand side the two factors are just the generating function at $x - 1$ and at $x + 1$ times an extra factor of z. The Fourier transform then converts these shifts of ± 1 in the spatial argument to the phase factors $e^{\pm ik}$, respectively. These steps give

$$\begin{aligned} P(k, z) - \sum_{x=-\infty}^{\infty} P(x, N = 0) e^{ikx} &= z(pe^{ik} + qe^{-ik}) P(k, z). \\ &\equiv zu(k)P(k, z), \end{aligned} \tag{1.3.3}$$

where $u(k)$ is the Fourier transform of the single-step hopping probability. For our biased nearest-neighbor random walk, $u(k)$ is $u(k) = pe^{ik} + qe^{-ik}$. The subtracted term on the left-hand side of Eq. (1.3.3) compensates for the absence of a term of the order of z^0 in Eq. (1.3.2). Thus for the initial condition of a particle initially at the origin, $P(x, N = 0) = \delta_{x,0}$, the joint Fourier transform and generating function of the probability distribution becomes

$$P(k, z) = \frac{1}{1 - zu(k)}. \tag{1.3.4}$$

We can now reconstruct the original probability distribution by inverting these transforms. When $P(k, z)$ is expanded in a Taylor series in z, the inverse of the generating function is simply $P(k, N) = u(k)^N$. Then the inverse Fourier transform is

$$P(x, N) = \frac{1}{2\pi} \oint e^{-ikx} u(k)^N \, dk, \tag{1.3.5}$$

where the integration is around the unit circle in the complex plane. To evaluate the integral, we write $u(k)^N = (pe^{ik} + qe^{-ik})^N$ in a binomial series. This

gives

$$P(x,N) = \frac{1}{2\pi}\oint e^{-ikx}\sum_{m=0}^{N}\binom{N}{m}p^m e^{ikm}q^{N-m}e^{-ik(N-m)}\,dk. \quad (1.3.6)$$

The only term that survives the integration is the one in which all the phase factors cancel. This is the term with $m = (N+x)/2$ and this ultimately leads to gives the classical binomial probability distribution of a discrete random walk:

$$P(x,N) = \frac{N!}{\left(\frac{N+x}{2}\right)!\left(\frac{N-x}{2}\right)!}\,p^{\frac{N+x}{2}}q^{\frac{N-x}{2}}. \quad (1.3.7)$$

Finally, using Stirling's approximation, this binomial approaches the Gaussian probability distribution in the long-time limit,

$$P(x,N) \to \frac{1}{\sqrt{2\pi Npq}}e^{-(x-Np)^2/2Npq}. \quad (1.3.8)$$

In fact, a Gaussian distribution arises for *any* hopping process in which the mean displacement $\langle x\rangle$ and the mean-square displacement $\langle x^2\rangle$ in a single step of the walk is finite. This is the statement of the *central-limit theorem* (Gnedenko and Kolmogorov (1954)). When $\langle x\rangle$ and $\langle x^2\rangle$ are both finite, $u(k)$ has the small-k series representation

$$u(k) = 1 + ik\langle x\rangle - \frac{1}{2}k^2\langle x^2\rangle + \ldots,$$
$$\sim e^{ik\langle x\rangle - \frac{1}{2}k^2\langle x^2\rangle}, \quad k \to 0.$$

When this result for $u(k)$ is substituted into Eq. (1.3.5), the main contribution to the integral comes from the region $k \to 0$. We can perform the resulting Gaussian integral by completing the square in the exponent; this leads to a Gaussian form for the probability distribution of a general nonsingular hopping process:

$$P(x,N) \to \frac{1}{\sqrt{2\pi N\langle x^2\rangle}}e^{-(x-\langle x\rangle)^2/2N\langle x^2\rangle}. \quad (1.3.9)$$

This independence of the probability distribution on details of the single-step hopping is a manifestation of the central-limit theorem. It is akin to the universality hypothesis of critical phenomena in which short-range details of a system do not affect large-scale properties [Stanley (1971)]. This same type of universality typifies random walks with short-range memory and/or correlations. The only property that is relevant is that $\langle x\rangle$ and $\langle x^2\rangle$ are both

finite. All such processes can be universally described by diffusion in the long-time limit.

As a complement to the above solution, which is based on $P(k, z) \to P(k, N) \to P(x, N)$, we first invert the Fourier transform in Eq. (1.3.4) to obtain the generating function for the occupation probability and then invert the latter to obtain the probability distribution; that is, we follow $P(k, z) \to P(x, z) \to P(x, N)$. This is conceptually identical to, although technically more complicated than, the inversion in the reverse order. However, there are applications in which the generating function $P(x, z)$ is indispensable (see Chap. 3) and it is also useful to understand how to move easily between generating functions, Laplace transforms, and real-time quantities. More on this will be presented in Section 1.4.

Starting with $P(k, z)$ in Eq. (1.3.4), the inverse Fourier transform is

$$P(x, z) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{e^{-ikx}}{1 - z(pe^{ik} + qe^{-ik})}\, dk. \tag{1.3.10}$$

We may perform this integral by introducing the variable $w = e^{-ik}$ to recast Eq. (1.3.10) as a contour around the unit circle in the complex plane. By applying basic methods from residue calculus, the value of the integral is

$$P(x, z) = \frac{1}{\sqrt{1 - 4pqz^2}} \left[\frac{1 - \sqrt{1 - 4pqz^2}}{2zq} \right]^{|x|}. \tag{1.3.11}$$

Finally, we may invert this generating function formally by again applying residue calculus to give the basic inversion formula

$$P(x, N) = \frac{1}{2\pi i} \oint \frac{P(x, z)}{z^{N+1}}\, dz, \tag{1.3.12}$$

where the clockwise contour encloses only the pole at the origin. We could also attempt to compute the power-series representation of $P(x, z)$ to arbitrary order to extract the original probability distribution. Neither approach appears to be elementary, however. This shows that the order of inverting the double transform $P(k, z)$ can be important: Here $P(k, z) \to P(k, N) \to P(x, N)$ is easy, whereas $P(k, z) \to P(x, z) \to P(x, N)$ is not. This is a useful lesson to keep in mind whenever one is dealing with combined Fourier–Laplace transforms.

1.3.2. Discrete Space and Continuous Time

For this representation, we replace the discrete time N and time increment $N \to N + 1$ with continuous time t and infinitesimal increment $t \to t + \delta t$

and Taylor expand the resulting master equation (1.3.1) to first order in δt. We also rewrite the spatial argument as the integer n to emphasize its discrete nature. These steps give

$$\frac{\partial P(n,t)}{\delta t} = w_+ P(n-1,t) + w_- P(n+1,t) - w_0 P(n,t), \quad (1.3.13)$$

where $w_+ = p/\delta t$ and $w_- = q/\delta t$ are the hopping rates to the right and to the left, respectively, and $w_0 = 1/\delta t$ is the total hopping rate from each site. This hopping process satisfies detailed balance, as the total hopping rates *to* a site equal the hopping rate *from* the same site.

By Fourier transforming, this master equation becomes an ordinary differential equation for the Fourier-transformed probability distribution

$$\begin{aligned} \frac{dP(k,t)}{dt} &= (w_+ e^{-ik} + w_- e^{ik} - w_0)\, P(k,t), \\ &\equiv w(k)\, P(k,t). \end{aligned} \quad (1.3.14)$$

For the initial condition $P(n, t=0) = \delta_{n,0}$, the corresponding Fourier transform is $P(k, t=0) = 1$, and the solution to Eq. (1.3.14) is simply $P(k,t) = e^{w(k)t}$. To invert this Fourier transform, it is useful to separate $w(k)$ into symmetric and antisymmetric components by defining $w_\pm \equiv \frac{1}{2} w_0 \pm \delta w$ to give $w(k) = w_0(\cos k - 1) - 2i\delta w \sin k$, and then use the generating function representations for the Bessel function [Abramowitz & Stegun (1972)],

$$\begin{aligned} e^{z\cos k} &= \sum_{n=-\infty}^{\infty} e^{ikn} I_n(z), \\ e^{z\sin k} &= \sum_{n=-\infty}^{\infty} (-i)^n e^{ikn} I_n(z), \end{aligned}$$

where $I_n(z)$ is the modified Bessel function of the first kind of order n. After some simple steps, we find

$$P(k,t) = e^{-w_0 t} \sum_{\ell,m=-\infty}^{\infty} (-i)^m\, e^{ik(\ell+m)}\, I_\ell(w_0 t)\, I_m(2i\delta w t). \quad (1.3.15)$$

By extracting the coefficient of e^{ikn} in this double series, we obtain

$$P(n,t) = e^{-w_0 t} \sum_{m=-\infty}^{\infty} (-i)^{n-m}\, I_m(w_0 t)\, I_{n-m}(2i\delta w t). \quad (1.3.16)$$

In particular, for the symmetric nearest-neighbor random walk, where $w_+ = w_- = w_0/2 = 1/2$, this reduces to the much simpler form

$$P(n,t) = e^{-t} I_n(t). \quad (1.3.17)$$

In this discrete-space continuous-time representation, the asymptotic behavior may be conveniently obtained in the limit of $t \to \infty$, but with n *fixed*. For example, the probability that site n is occupied, as $t \to \infty$, is

$$P(n,t) = \frac{1}{\sqrt{2\pi t}}\left[1 - \frac{4n^2-1}{8t} + \cdots\right]. \tag{1.3.18}$$

This gives the well-known result that the probability for a random walk to remain at the origin vanishes as $t^{-1/2}$. However, this discrete-space and continuous-time representation is awkward for determining the Gaussian scaling behavior of occupation probability, in which n and t both diverge but n^2/t remains constant. For this limit, the continuum formulation is much more appropriate.

To determine the probability distribution in this interesting scaling limit, we introduce the Laplace transform of the probability distribution $P(n,s) = \int_0^\infty e^{-st}\, P(n,t)\, dt$ and for simplicity consider the symmetric random walk. Applying this Laplace transform to master equation (1.3.13) then gives

$$\int_0^\infty dt\, e^{-st}\left[\frac{\partial P(n,t)}{\partial t} = \frac{1}{2}P(n+1,t) + \frac{1}{2}P(n-1,t) - P(n,t)\right].$$

This Laplace transform reduces the master equation to the discrete recursion formula

$$sP(n,s) - P(n,t=0) = \frac{1}{2}P(n+1,s) + \frac{1}{2}P(n-1,s) - P(n,s). \tag{1.3.19}$$

For $n \neq 0$, we have $P(n,s) = a[P(n+1,s) + P(n-1,s)]$, with $a = 1/2(s+1)$. We solve this difference equation by assuming the exponential solution $P(n,s) = A\lambda^n$ for $n > 0$. For the given initial condition, the solution is symmetric in n; hence $P(n,s) = A\lambda^{-n}$ for $n < 0$. Substituting this form into the recursion for $P(n,s)$ gives a quadratic characteristic equation for λ whose solution is $\lambda_\pm = (1 \pm \sqrt{1-4a^2})/2a$. For all $s > 0$, $\lambda_\pm$ are both real and positive, with $\lambda_+ > 1$ and $\lambda_- < 1$. For regularity at $n = \infty$, we must reject the solution that grows exponentially with n, thus giving $P_n = A\lambda_-^n$. Finally, we obtain the constant A from the $n = 0$ boundary master equation:

$$\begin{aligned} sP(0,s) - 1 &= \frac{1}{2}P(1,s) + \frac{1}{2}P(-1,s) - P(0,s) \\ &= P(1,s) - P(0,s). \end{aligned} \tag{1.3.20}$$

The -1 on the left-hand side arises from the initial condition, and the second equality follows by spatial symmetry. Substituting $P(n,s) = A\lambda_-^n$ into

Eq. (1.3.20) gives A, from which we finally obtain

$$P(n,s) = \frac{1}{s+1-\lambda_-}\,\lambda_-^n. \tag{1.3.21}$$

This Laplace transform diverges at $s = 0$; consequently, we may easily obtain the interesting asymptotic behavior by considering the limiting form of $P(n,s)$ as $s \to 0$ limit. Because $\lambda_- \approx 1 - \sqrt{2s}$ as $s \to 0$, we find

$$\begin{aligned} P(n,s) &\approx \frac{(1-\sqrt{2s})^n}{\sqrt{2s}+s} \\ &\sim \frac{e^{-n\sqrt{2s}}}{\sqrt{2s}}. \end{aligned} \tag{1.3.22}$$

We can now compute the inverse Laplace transform $P(n,t) = \int_{s_0-i\infty}^{s_0+i\infty} P(n,s)e^{st}\,ds$ by elementary means by using the integration variable $u = \sqrt{s}$. This immediately leads to the Gaussian probability distribution quoted in Eq. (1.3.9) for the case $\langle x\rangle = 0$ and $\langle x^2\rangle = 1$.

1.3.3. Continuous Space and Time

Finally, consider master equation (1.3.1) in both continuous time and space. By expanding this equation in a Taylor series to lowest nonvanishing order – second order in space x and first order in time t – we obtain the fundamental *convection–diffusion equation*,

$$\frac{\partial c(x,t)}{\partial t} + v\frac{\partial c(x,t)}{\partial x} = D\,\frac{\partial^2 c(x,t)}{\partial x}, \tag{1.3.23}$$

for the particle concentration $c(x,t)$. This should be viewed as the continuum analog of the occupation probability of the random walk; we will therefore use $c(x,t)$ and $P(x,t)$ interchangeably. Here $v = (p-q)\delta x/\delta t$ is the bias velocity and $D = \delta x^2/2\delta t$ is the diffusion coefficient. For the symmetric random walk, the probability distribution obeys the simpler *diffusion equation*

$$\frac{\partial c(x,t)}{\partial t} = D\,\frac{\partial^2 c(x,t)}{\partial x}. \tag{1.3.24}$$

Note that in the convection–diffusion equation, the factor v/D diverges as $1/\delta x$ in the continuum limit. Therefore the convective term $\partial c/\partial x$ invariably dominates over the diffusion term $\partial^2 c/\partial x^2$. To construct a nonpathological continuum limit, the bias $p-q$ must be proportional to δx as $\delta x \to 0$ so that both the first- and the second-order spatial derivative terms are simultaneously finite. For the diffusion equation, we obtain a nonsingular continuum limit

merely by ensuring that the ratio $\delta x^2/\delta t$ remains finite as both δx and δt approach zero. Roughly speaking, any stochastic hopping process in which the distribution of step lengths is well behaved has a continuum description in terms of the convection–diffusion or the diffusion equation. Much more about this relation between discrete hopping processes and the continuum can be found, for example, in Gardiner (1985), Weiss (1994), or van Kampen (1997).

Several basic approaches are now given for solving the diffusion and the convection–diffusion equations.

1.3.3.1. Scaling Solution

Scaling provides a relatively cheap but general approach for solving wide classes of partial differential equations that involve diverging characteristic scales, such as coarsening, aggregation, fragmentation, and many other nonequilibrium processes [see, e.g., Lifshitz & Slyozov (1961), Ernst (1985), and Cheng & Redner (1990) for examples of each]. For the diffusion equation, the scaling solution is based on the observation that there is a *single* length scale that characterizes the particle displacement. Consequently, the probability density is not a function of x and t separately, but rather, is a function of the scaling variable $u \equiv x/X(t)$, where $X(t)$ is the characteristic length scale of the spatial spread of the probability distribution. We may then separate the dependences on u and t to give two single-variable equations – one for the time dependence and another for the functional form of the probability distribution. For the convection–diffusion equation, two length scales are needed to characterize the probability distribution, and, although a scaling approach is still tractable, it no longer has the same degree of simplicity.

The scaling ansatz for the concentration in the diffusion equation is

$$c(x,t) = \frac{1}{X(t)} f[x/X(t)]. \tag{1.3.25}$$

The prefactor $1/X(t)$ ensures that the spatial integral of $c(x,t)$ is normalized, $\int c(x,t)\,dx = 1$, as is evident by dimensional analysis, and the function f encodes the dependence on the scaled distance $u = x/X(t)$. Substituting this ansatz into the diffusion equation gives, after some elementary algebra,

$$X(t)\dot{X}(t) = -D\frac{f''(u)}{f(u) + uf'(u)}, \tag{1.3.26}$$

where the prime denotes differentiation with respect to u and the overdot denotes the time derivative. Because the left-hand side is a function of time only whereas the right-hand side is a function of u only, both sides must equal

a constant. The scaling ansatz thus leads to variable separation. Strikingly, the value of the separation constant drops out of the solution to the diffusion equation. However, in more complex situations, such as aggregation and coarsening, the separation constant plays an essential role in characterizing the solution, and additional physical considerations must be imposed to determine the solution completely. These are beyond the scope of the present discussion.

Solving for the time dependence gives $X\dot{X} = A$, or $X(t)^2 = 2At$. When this is used in Eq. (1.3.26), the scaling function satisfies

$$f'' = -\frac{A}{D}(f + uf') = -\frac{A}{D}(uf)'.$$

Integrating once gives $f' = -Auf/D + \text{const}$, but the symmetry condition $f' = 0$ at $u = 0$, which corresponds to the random walk starting at the origin, means that the constant is zero. Integrating once again gives the scaling function

$$f(u) = f(0)e^{-Au^2/2D},$$

where the prefactor $f(0)$ is most easily determined by invoking normalization. With $u = x/X(t)$, the final result for the concentration is

$$c(x,t) = \frac{1}{\sqrt{4\pi Dt}}\, e^{-x^2/4Dt}, \tag{1.3.27}$$

where, as advertised, the separation constant A drops out of this solution. Note that for $D = 1/2$ this solution agrees with expression (1.3.9), with $\langle x^2 \rangle = 1$ and $N \to t$.

1.3.3.2. *Fourier Transform Solution*

Here we solve the convection–diffusion equation by first introducing the Fourier transform

$$c(k,t) = \int c(x,t)\, e^{ikx}\, dx$$

to simplify the convection–diffusion equation to

$$\dot{c}(k,t) = (ikv - Dk^2)c(k,t). \tag{1.3.28}$$

The solution is

$$\begin{aligned} c(k,t) &= c(k,0)e^{(ikv - Dk^2)t} \\ &= e^{(ikv - Dk^2)t} \end{aligned} \tag{1.3.29}$$

for the initial condition $c(x, t = 0) = \delta(x)$. We then obtain the probability distribution by the inverse Fourier transform

$$c(x, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{(ikv - Dk^2)t - ikx}\, dk.$$

We may perform this integral by completing the square in the exponential, and the final result is the Gaussian probability distribution

$$c(x, t) = \frac{1}{\sqrt{4\pi Dt}}\, e^{-(x-vt)^2/4Dt}. \tag{1.3.30}$$

1.3.3.3. Laplace Transform Solution

An alternative approach is to first perform a Laplace transform in the time domain. For the convection–diffusion equation, this yields the ordinary differential equation

$$sc(x, s) - \delta(x) + vc(x, s) = Dc''(x, s), \tag{1.3.31}$$

where the delta function again reflects the initial condition of a particle at the origin at $t = 0$. This equation may be solved separately in the half-spaces $x > 0$ and $x < 0$. In each subdomain Eq. (1.3.31) reduces to a homogeneous constant-coefficient differential equation that has exponential solutions in x. The corresponding solution for the entire line has the form $c_+(x, s) = A_+ e^{-\alpha_+ x}$ for $x > 0$ and $c_-(x, s) = A_- e^{\alpha_+ x}$ for $x < 0$, where $\alpha_\pm = (v \pm \sqrt{v^2 + 4Ds})/2D$ are the roots of the characteristic polynomial. The complementary divergent term in each of these half-space solutions has been discarded. When these two solutions are joined at the origin, they yield the global solution. The appropriate joining conditions are continuity of $c(x, s)$ at $x = 0$, and a discontinuity in $(\partial c/\partial x)$ at $x = 0$ whose magnitude is determined by integrating Eq. (1.3.31) over an infinitesimal domain that includes the origin.

The continuity condition trivially gives $A_+ = A_- \equiv A$, and the condition for the discontinuity in $c(x, s)$ is

$$D(c'_+|_{x=0} - c'_-|_{x=0}) = -1.$$

This gives $A = 1/\sqrt{v^2 + 4Ds}$. Thus the Laplace transform of the probability distribution is

$$c_\pm(x, s) = \frac{1}{\sqrt{v^2 + 4Ds}}\, e^{-\alpha_+ |x|}. \tag{1.3.32}$$

For zero bias, this coincides with Eq. (1.3.22) and thus recovers the Gaussian probability distribution.

1.3.3.4. Fourier–Laplace Transform Solution

Perhaps the simplest approach for solving the convection–diffusion equation is to apply the combined Fourier–Laplace transform

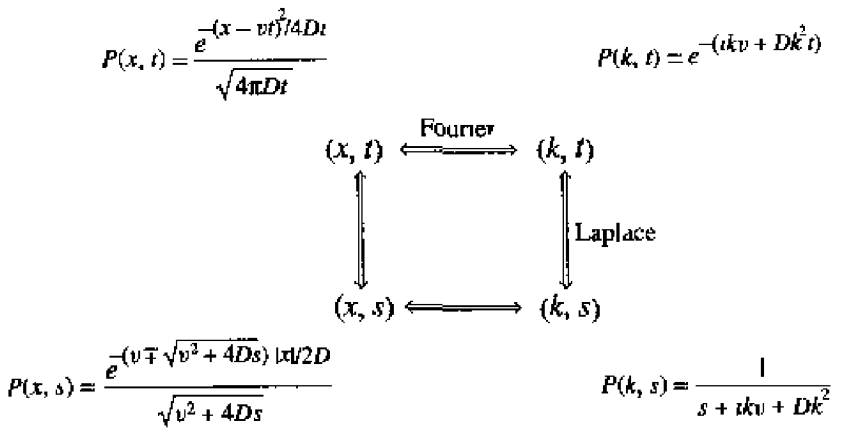
$$c(k, s) = \int_{-\infty}^{\infty} dx\, e^{ikx} \int_0^{\infty} dt\, c(x, t) e^{-st}$$

to recast the differential equation into the purely algebraic equation $sc(k, s) - 1 = -(ivk + Dk^2)c(k, s)$. The solution to the latter is

$$c(k, s) = \frac{1}{s + ivk + Dk^2}. \tag{1.3.33}$$

Performing the requisite inverse transforms, we again recover the Gaussian probability distribution as a function of space and time.

In summary, all of the representations of the probability distribution for the convection–diffusion equation are interrelated and equivalent, as represented graphically below. The nature of the problem usually dictates which representation is best to use in solving a specific problem.



1.4. Relation between Laplace Traasforms and Real-Time Quantities

In first-passage phenomena, we typically seek the asymptotic behavior of a time-dependent quantity when only its generating function or its Laplace transform is readily available. A typical example is a function $F(t)$ whose generating function has the form $F(z) \sim (1 - z)^{\mu - 1}$, with $\mu < 1$ as $z \to 1$ from below. We will show that the corresponding time dependence is $F(t) \sim t^{-\mu}$ as $t \to \infty$. Although there are well-established and rigorous methods available for inverting such transforms [see, e.g., Titschmarsh (1945), Hardy (1947), and the discussion in Weiss (1994) for specific applications to random walks], if we are interested in long-time properties only, then basic asymptotic features can be gained through simple and intuitively appealing means. Although lacking in rigor, they provide the correct behavior for all cases

of physical interest. The most useful of these methods are outlined in this section.

Let us first determine the long-time behavior of a function $F(t)$ when only the associated generating function $F(z) = \sum_{t=0}^{\infty} F(t) z^t$ is available. There are two fundamentally different cases: (a) $\sum_{t=0}^{\infty} F(t)$ diverges or (b) $\sum_{t=0}^{\infty} F(t)$ converges.

We relate the generating function $F(z)$ to $F(t)$ by the following steps:

$$\begin{aligned} F(z) &= \sum_{t=0}^{\infty} F(t) z^t \\ &\approx \int^{\infty} F(t) e^{-t \ln(1/z)}\, dt \\ &\sim \int^{t^*} F(t)\, dt, \end{aligned} \tag{1.4.1}$$

with $t^* = [\ln(1/z)]^{-1}$. These simple algebraic steps involve several important simplifications and approximations that we can justify as follows:

- Converting the sum to an integral. In many cases of relevance to first-passage phenomena, $F(t) \sim t^{-\mu}$ for $t \to \infty$ but rapidly goes to zero for $t \to 0$. Further, it is usually only the long-time behavior of $F(t)$ that is readily obtainable in the continuum limit. If we were to use the continuum expression for $F(t)$ in the integral for all times, a spurious singularity could arise from the contribution to the integral at short times. We eliminate this unphysical singularity by replacing the lower limit with a value of the order of 1. Because asymptotic behavior is unaffected by this detail, we often leave the lower limit as indefinite with the understanding that it is of the order of 1.
- From the second line of Eq. (1.4.1), we see that $F(z)$ is essentially the Laplace transform of $F(t)$ with $s = \ln(1/z)$. Because the $s \to 0$ limit of the Laplace transform corresponds to long-time limit of $F(t)$, we immediately infer that long-time behavior may also be obtained from the limit $z \to 1$ from below in the generating function.
- Sharp cutoff. In the last step, we replace the exponential cutoff in the integral, with characteristic lifetime $t^* = [\ln(1/z)]^{-1}$, with a step function at t^*. Although this crude approximation introduces numerical errors of the order of 1, we shall see that the essential asymptotic behavior is preserved when $\sum_{t=0}^{\infty} F(t)$ diverges.

We now use the approach of Eq. (1.4.1) to determine the asymptotic relation between $F(t)$ and $F(z)$, considering separately the two fundamental cases in which $\sum_{t=0}^{\infty} F(t)$ diverges and in which it converges. In the former case, it is

natural to use $s \equiv (1 - z)$ as the basic variable, since the generating function diverges as $z \to 1$. Then $t^* = [\ln(1/z)]^{-1} \sim 1/s$ for small s. Thus the basic relation between $F(t)$ and $F(z)$ is simply

$$F(z) \sim \int^{1/s} F(t)\,dt. \tag{1.4.2}$$

Now if $F(t) \to t^{-\mu}$ with $\mu < 1$ as $t \to \infty$, then $F(z)$ diverges as

$$F(z) \sim \int^{1/s} t^{-\mu}\,dt \sim s^{\mu-1} = (1 - z)^{\mu-1} \tag{1.4.3}$$

as $z \to 1$ from below. In summary, the fundamental connection is

$$F(t) \sim t^{-\mu} \longleftrightarrow F(z) \sim (1 - z)^{\mu-1}. \tag{1.4.4}$$

As a useful illustration of the equivalence between the generating function as $z \to 1$ from below and the Laplace transform, let us reconsider the formidable-looking generating function of the one-dimensional random walk

$$P(x, z) = \frac{1}{\sqrt{1 - z^2}} \left[\frac{1 - \sqrt{1 - z^2}}{z}\right]^{|x|}. \tag{1.4.5}$$

By taking the limit $z \to 1$ from below, we obtain

$$\begin{aligned} P(x, z) &\approx \frac{[1 - \sqrt{2(1 - z)}]^{|x|}}{\sqrt{2(1 - z)}} \\ &\sim \frac{e^{-x\sqrt{2s}}}{\sqrt{2s}}, \quad \text{letting } s = 1 - z. \end{aligned} \tag{1.4.6}$$

which reproduces the Laplace transform in approximation (1.3.22).

Parenthetically, another useful feature of the generating function is that it can simplify integral relations between two functions of the generic form $P(t) = \sum_{t'=0}^{t} F(t')$. By introducing the generating functions for P and F, we easily obtain the corresponding relation between the generating functions $P(z) = F(z)/(1 - z)$. In continuous time, the corresponding relation $P(t) = \int_0^t F(t')\,dt'$ translates to $P(s) = F(s)/s$ for the Laplace transforms.

Finally, let us discuss the general connection between the time integral of a function, $\mathcal{F}(t) \equiv \int_0^t F(t)\,dt$, and the generating function $F(z)$. For $z = 1 - 1/t^*$ with $t^* \to \infty$, approximation (1.4.2) becomes

$$F(z = 1 - 1/t^*) \sim \int_0^{t^*} F(t)\,dt = \mathcal{F}(t^*). \tag{1.4.7}$$

Thus a mere variable substitution provides an approximate, but asymptotically correct, algebraic relation between the generating function (or Laplace

transform) and the time integral of the function itself. For this class of examples, there is no need to perform an integral to relate a function and its Laplace transform.

Conversely, when $\sum_t^\infty F(t)$ converges, the simplifications outlined in Eq. (1.4.1) no longer apply and we must be more careful in constructing the relation between $F(t)$ and $F(z)$. We again suppose that $F(t) \sim t^{-\mu}$ as $t \to \infty$, but now with $\mu > 1$ so that $F(z)$ is finite as $z = 1$. Then $F(z)$ typically has the form $F(z) = F(1) + p_1(1-z)^{\alpha_1} + \cdots$ as $z \to 1$, where p_1 is a constant. To determine the exponent α_1 in the first correction term, consider the difference $F(1) - F(z)$. We again use $z = 1 - s$ when $z \to 1$, so that

$$\begin{aligned} F(1) - F(z) &\propto \sum_t^\infty t^{-\mu}(1 - z^t), \\ &\sim \int^\infty t^{-\mu}(1 - e^{-st})\, dt, \\ &\sim \int_{1/s}^\infty t^{-\mu}\, dt, \\ &\sim (1-z)^{\mu-1}. \end{aligned} \tag{1.4.8}$$

The exponential cutoff in the integrand has again been replaced with a sharp cutoff at $t = 1/s$ in the third line. We therefore infer the asymptotic behavior

$$F(z) \sim F(1) + a_1(1-z)^{\mu-1} + \ldots, \tag{1.4.9}$$

where the a_1 is a detail-dependent constant.

Parallel results exist for the Laplace transform. For a generic power-law form, $F(t) \sim t^{-\mu}$, the Laplace transform $F(s)$ has the small-s expansion:

$$F(s) \sim F(s=0) + (A_1 s^\alpha + A_2 s^{\alpha+1} + \cdots) + (B_1 s^1 + B_2 s^2 + \cdots). \tag{1.4.10}$$

There are again several possibilities. When $\mu \neq 1$, asymptotic behavior is governed by the nonanalytic term. In this case, the exponent $\alpha = \mu - 1$. Note also that when α is less than one, then the first moment and indeed all positive integer moments of $F(t)$ are divergent. This is reflected by the fact that $F(t)$ has the power-law tail $t^{-\mu}$ with $\mu = \alpha + 1 < 2$. Additionally, note that the zeroth-order term in Eq. (1.4.9) is $\int_0^\infty F(t)\, dt$. Thus if $F(t)$ is the first-passage probability to a given point, $F(s=0)$ is the probability of *eventually* hitting this point.

On the other hand, if all positive moments of $F(t)$,

$$\langle t^n \rangle = \frac{\int_0^\infty t^n\, F(t)\, dt}{\int_0^\infty F(t)\, dt}, \tag{1.4.11}$$

exist, then $F(s)$ in Eq. (1.4.10) contains only the Taylor series terms. These generate the positive integer moments of $F(t)$ by means of

$$\begin{aligned} F(s) &= \int_0^\infty F(t) e^{-st}\, dt \\ &= \int_0^\infty F(t) \left(1 - st + \frac{s^2 t^2}{2!} - \frac{s^3 t^3}{3!} + \cdots\right) \\ &= \mathcal{F}(\infty) \left(1 - s\langle t\rangle + \frac{s^2}{2!}\langle t^2\rangle - \frac{s^3}{3!}\langle t^3\rangle + \cdots\right). \end{aligned} \tag{1.4.12}$$

Thus the Laplace transform is a *moment generating function*, as it contains *all* the positive integer moments of the probability distribution $F(t)$. This is one of the reasons why the Laplace transform is such a useful tool for first-passage processes.

In summary, the small-s behavior of the Laplace transform, or, equivalently, the $z \to 1$ behavior of the generating function, are sufficient to determine the long-time behavior of the function itself. Because the transformed quantities are usually easy to obtain by the solution of an appropriate boundary-value problem, the asymptotic methods outlined here provide a simple route to obtain long-time behavior.

1.5. Asymptotics of the First-Passage Probability

We now use the techniques of Section 1.4 to determine the time dependence of the first-passage probability in terms of the generating function for the occupation probability. For simplicity, consider an isotropic random walk that starts at the origin. From the Gaussian probability distribution given in Eq. (1.3.27), $P(\vec{r} = 0, t) = (4\pi Dt)^{-d/2}$ in d dimensions. Then Eq. (1.4.1) gives the corresponding generating function:

$$P(0, z) \approx \int^\infty P(0, t)\, z^t\, dt \sim \int^\infty (4\pi Dt)^{-d/2} z^t\, dt. \tag{1.5.1}$$

As discussed in Section 1.4, this integral has two fundamentally different behaviors, depending on whether $\int^\infty P(0, t)\, dt$ diverges or converges. In the

former case, we apply the last step in Eq. (1.4.1) to obtain

$$P(0,z) \propto \int^{t^*} (4\pi Dt)^{-d/2}\, dt \sim \begin{cases} A_d (t^*)^{1-d/2} = A_d (1-z)^{d/2-1}, & d < 2 \\ A_2 \ln t^* = -A_2 \ln(1-z), & d = 2 \end{cases}, \tag{1.5.2}$$

where the dimension-dependent prefactor A_d is of the order of 1 and does not play any role in the asymptotic behavior,

For $d > 2$, the integral $\int^{\infty} P(0,t)\, dt$ converges and we apply Eq. (1.4.8) to compute the asymptotic behavior of $P(0,1) - P(0,z)$. By definition, $F(0,1) = \sum_t F(0,t) = 1 - [P(0,1)]^{-1}$. Further, $\sum_t F(0,t)$ is just the eventual probability $\mathcal{R}$ that a random walk reaches the origin, so that $P(0,1) = (1-\mathcal{R})^{-1}$. In the asymptotic limit $z = 1 - s$, with $s \to 0$, $P(0,1) - P(0,z)$ may therefore be written as

$$\begin{aligned} P(0,1) - P(0,z) &\propto \sum_{t=1}^{\infty} t^{-d/2}(1 - z^t), \\ &\sim (1-z)^{d/2-1}. \end{aligned} \tag{1.5.3}$$

Thus $P(0,z)$ has the asymptotic behavior

$$P(0,z) \sim (1-\mathcal{R})^{-1} + B_d (1-z)^{d/2-1} + \ldots, \quad d > 2, \tag{1.5.4}$$

where B_d is another dimension-dependent constant of the order of 1. Using these results in Eq. (1.2.3), we infer that the generating function for the first-passage probability has the asymptotic behaviors

$$F(0,z) = 1 - \sqrt{1-z^2}, \quad d = 1, \tag{1.5.5}$$

whereas, for $d > 1$,

$$F(0,z) \sim \begin{cases} 1 - \dfrac{1}{A_d (1-z)^{d/2-1}}, & d < 2 \\ 1 + \dfrac{1}{A_2 \ln(1-z)}, & d = 2 \\ \mathcal{R} + B_d (1-R)^2 (1-z)^{d/2-1}, & d > 2 \end{cases}. \tag{1.5.6}$$

From this generating function, we determine the time dependence of the survival probability by approximation (1.4.7); that is,

$$\begin{aligned} F(0, z = 1 - 1/t^*) &\sim \int_0^{t^*} F(0,t)\, dt \\ &= \text{first-passage probability up to time } t^* \\ &\equiv T(t^*) = 1 - S(t^*), \end{aligned} \tag{1.5.7}$$

where $S(t)$ is the survival probability and $T(t)$ is the complementary probability that the particle is trapped, that is, reaches the origin by time t. From Eqs. (1.5.6) and (1.5.7) we thus find

$$S(t) \sim \begin{cases} \dfrac{1}{A_d t^{1-d/2}}, & d < 2 \\ \dfrac{1}{A_2 \ln t}, & d = 2 \\ (1-\mathcal{R}) + C_d(1-\mathcal{R})^2 t^{1-d/2}, & d > 2 \end{cases} \tag{1.5.8}$$

where C_d is another d-dependent constant of the order of 1. Finally, the time dependence of the first-passage probability may be obtained from the basic relation $1 - S(t) \sim \int^t F(0,t)\,dt$ to give

$$F(0,t) = -\frac{\partial S(t)}{\partial t} \propto \begin{cases} t^{d/2-2}, & d < 2 \\ \dfrac{1}{t \ln^2 t}, & d = 2 \\ t^{-d/2}, & d > 2 \end{cases} . \tag{1.5.9}$$

Equations (1.5.8) and (1.5.9) are the fundamental results of this section – the asymptotic time dependences of the survival and the first-passage probabilities. There are several important features that deserve emphasis. First, asymptotic time dependence is determined by the spatial dimension only, and not on any other properties of diffusive motion. Note, in particular, the change in behavior as a function of spatial dimension. For $d \leq 2$, the survival probability $S(t)$ ultimately decays to zero. This means that a random walk is *recurrent*, that is, certain to eventually return to its starting point, and indeed visit *any* site of an infinite lattice. Finally, because a random walk has no memory, it is "renewed" every time a specific lattice site is reached. Thus recurrence also implies that every site is visited infinitely often.

There is a simple physical basis for this efficient visitation of lattice sites. After a time t, a random walk explores a roughly spherical domain of radius $\sqrt{Dt}$. The total number of sites visited during this exploration is also proportional to t. Consequently, in d dimensions, the density of visited sites within this exploration sphere is $\rho \propto t/t^{d/2} \propto t^{1-d/2}$. Because this diverges as $t \to \infty$ for $d < 2$, a random walk visits each site within the sphere infinitely often; this is termed *compact exploration* [de Gennes (1983)]. Paradoxically, although every site is visited with certainty, these visitations take forever because the mean time to return to the origin, $\langle t \rangle = \int t F(0,t)\,dt$, diverges for all $d \leq 2$.

On the other hand, for $d > 2$, Eq. (1.5.8) predicts that there is a nonzero probability for a diffusing particle to not return to its starting point. More

generally, there is a nonzero probability for a random walk to miss most of the lattice sites. This incomplete visitation follows from the density of visited sites ρ within the exploration sphere tending to zero as $t \to \infty$. Thus the random-walk trajectory within this sphere is relatively "transparent." This behavior is more commonly known as *transient* [Pólya (1921) and Feller (1968)].

The distinction between recurrence and transience has important physical implications. As a basic example, consider a diffusion-controlled reaction in three dimensions. Because the trajectory of each diffusing reactant is transparent, the probability for two molecules to meet is essentially independent of their initial separation. This means that a molecule reacts with any other reactant molecule in the system with almost equal probability. Such an egalitarian process corresponds to the mean-field limit. Conversely, for dimension $d \leq 2$, nearby reactants are most likely to meet and this naturally induces slow kinetics and spatial correlations (see Chap. 8).

For a biased random walk, first-passage characteristics are largely dominated by the bias. For $d > 1$, a biased random walk visits only those lattice sites within a narrow cone along the bias whose length is proportional to t and whose width is proportional to $t^{1/2}$. The density of visited sites within this cone is therefore $t/t^{1+(d-1)/2} \sim t^{(1-d)/2}$. Thus a biased random walk is transient for all $d > 1$. For $d = 1$ there is a trivial version of recurrence in which each downstream site is visited with certainty, but only a finite number of times.

1.6. Connection between First-Passage and Electrostatics

1.6.1. Background

The fundamental connection between the first-passage properties of diffusion and electrostatics is now outlined. Basic questions of first passage include *where* a diffusing particle is absorbed on a boundary and *when* does this absorption event occur. These are *time-integrated* attributes, obtained by integration of a time-dependent observable over all time. For example, to determine when a particle is absorbed, we should compute the first-passage probability to the boundary and then integrate over all time to obtain the *eventual hitting probability*. However, it is more elegant to reverse the order of calculation and first integrate the equation of motion over time and then compute the outgoing flux at the boundary. This first step transforms the diffusion equation to the simpler Laplace equation. Then, in computing the flux, the exit probability is just the electric field at the boundary point. Thus there is

a complete correspondence between a first-passage problem and an electrostatic problem in the same geometry. This mapping is simple yet powerful, and can be adapted to compute related time-integrated properties, such as the splitting probabilities and the moments of the exit time. Some of these simplifications are also discussed in Gardiner (1985) and Risken (1988).

1.6.2. The Green's Function Formalism

Let us recall the conventional method to compute the first-passage probability of diffusion. Consider a diffusing particle that starts at $\vec{r}_0$ within a domain with boundary B. We compute the hitting probability to a point $\vec{r}_B$ on this boundary by first solving for the Green's function for the diffusion equation

$$\frac{\partial c(\vec{r}, t; \vec{r}_0)}{\partial t} = D\nabla^2 c(\vec{r}, t; \vec{r}_0), \tag{1.6.1}$$

with the initial condition $c(\vec{r}, 0; \vec{r}_0) = \delta(\vec{r} - \vec{r}_0)$ and the absorbing boundary condition $c(\vec{r}, t; \vec{r}_0)|_{\vec{r}\in B} = 0$. This condition accounts for the fact that once a particle reaches the boundary it leaves the system. Because the initial condition is invariably a single particle at $\vec{r}_0$, we will typically not write this argument in the Green's function. The outgoing flux at $\vec{r}_B$, $j(\vec{r}_B, t)$, is simply

$$j(\vec{r}_B, t) = -D\frac{\partial c(\vec{r}, t)}{\partial \hat{n}}\bigg|_{\vec{r}=\vec{r}_B}, \tag{1.6.2}$$

where $\hat{n}$ is a unit outward normal at $\vec{r}_B$. Finally, the eventual hitting probability at $\vec{r}_B$ is

$$\mathcal{E}(\vec{r}_B) = \int_0^\infty j(\vec{r}_B, t)\, dt. \tag{1.6.3}$$

In this direct approach, we first solve the diffusion equation, which has a first derivative in time, and then effectively "undo" the differentiation by integrating over all time to find the eventual hitting probability.

1.6.2.1. Hitting Probability

We now rederive this hitting probability by mapping the time-integrated diffusive system to electrostatics. First we integrate Eq. (1.6.1) over all time to give

$$c(\vec{r}, t = \infty) - c(\vec{r}, t = 0) = D\nabla^2 C_0(\vec{r}), \tag{1.6.4}$$

where $C_0(\vec{r}) = \int_0^\infty c(\vec{r}, t)\, dt$ is the time integral of the Green's function. (The reason for including the subscript 0 will become apparent shortly.) We now consider spatial domains for which eventual absorption is certain, that is, $c(\vec{r}, t = \infty) = 0$. Additionally, at $t = 0$ the Green's function just reduces to the initial condition $c(\vec{r}, t = 0) = \delta(\vec{r} - \vec{r}_0)$. Thus $C_0(\vec{r})$ obeys the Laplace equation

$$D\nabla^2 C_0(\vec{r}) = -\delta(\vec{r} - \vec{r}_0), \tag{1.6.5}$$

with homogeneous Dirichlet boundary conditions. This defines an electrostatic system with a point charge of magnitude $1/(D\Omega_d)$ at $\vec{r}_0$ (where Ω_d is the surface area of a d-dimensional unit sphere). The absorbing boundaries in the diffusive system are equivalent to grounded conducting surfaces in the corresponding electrostatic problem. More general initial conditions can easily be considered by the linearity of the basic equations.

In terms of C_0, the eventual hitting probability $\mathcal{E}(\vec{r}_B)$ is given by

$$\begin{aligned} \mathcal{E}(\vec{r}_B) &= \int_0^\infty j(\vec{r}_B, t) dt \\ &= -D \int_0^\infty \frac{\partial c(\vec{r}, t)}{\partial \hat{n}}\, dt \\ &= -D \frac{\partial C_0}{\partial \hat{n}}. \end{aligned} \tag{1.6.6}$$

On the other hand, from Eq. (1.6.5) this normal derivative is just the electric field associated with the initial charge distribution. This leads to the following fundamental conclusion:

- For a diffusing particle that is initially at $\vec{r}_0$ inside a domain with absorbing boundary conditions, the eventual hitting probability to a boundary point $\vec{r}_B$ equals the electric field at this same location when a point charge of magnitude $1/(D\Omega_d)$ is placed at $\vec{r}_0$ and the domain boundary is grounded.

This simplifies the computation of the exit probability significantly, as it is much easier to solve the time-independent Laplace equation rather than the corresponding diffusion equation.

1.6.2.2. Hitting Time

This electrostatic formalism can be extended to integer moments of the mean time to exit or hit the boundary. By definition, the nth moment of the exit

time is

$$\langle t^n \rangle = \int_0^\infty t^n F(t)\, dt, \tag{1.6.7}$$

where $F(t)$ is the first-passage probability to the boundary at time t. Here we are again tacitly considering situations for which the particle is certain to eventually reach the exit boundary. If $\langle t^0 \rangle = \int_0^\infty F(t)\, dt < 1$, as would occur if we were considering the first passage to a subset of a composite boundary, then the formulas given below need to be normalized in an obvious way by dividing the moments by $\langle t^0 \rangle$.

Using the fact that $F(t) = -[\partial S(t)/\partial t]$, we integrate by parts to obtain

$$\begin{aligned} \langle t^n \rangle &= -\int_0^\infty t^n \frac{\partial S(t)}{\partial t}\, dt, \\ &= -t^n S(t)\Big|_0^\infty + n \int_0^\infty t^{n-1} S(t)\, dt \\ &= n \int_0^\infty t^{n-1}\, dt \int_V c(\vec{r}, t)\, d\vec{r}. \end{aligned} \tag{1.6.8}$$

In the second line, the integrated term is trivially equal to zero at the lower limit and equals zero at the upper limit if the system is finite and $S(t) \to 0$ faster than a power law as $t \to \infty$. In the last line, the integral is over the domain volume. Note the important special case of $n = 1$ for which the mean exit time is simply $\langle t \rangle = \int_0^\infty S(t)\, dt$.

We now recast this derivation for $\langle t^n \rangle$ as a time-independent problem by reversing the order of the temporal and the spatial integrations at the outset. First, we define the time-integrated moments of the probability distribution

$$C_n(\vec{r}) = \int_0^\infty c(\vec{r}, t)\, t^n\, dt. \tag{1.6.9}$$

Then, from the last line of Eq. (1.6.8), the nth moment of the mean exit time is just the time-independent expression

$$\langle t^n \rangle = n \int_V C_{n-1}(\vec{r})\, d\vec{r}. \tag{1.6.10}$$

We now show that each of these integrated moments satisfies the Poisson equation with an n-dependent source term. Consider

$$\int_0^\infty t^n \left[\frac{\partial c(\vec{r}, t)}{\partial t} = D\nabla^2 c(\vec{r}, t) \right] dt. \tag{1.6.11}$$

Integrating the left-hand side by parts, we find that the integrated term,

$t^n c(\vec{r}, t)|_0^\infty$, vanishes, except for $n = 0$, where the lower limit coincides with the initial condition. The remaining term, $-\int_0^\infty n\, t^{n-1} c(\vec{r}, t)\, dt$, is proportional to the time-integrated moment of order $n - 1$. The right-hand side is just $D\nabla^2 C_n(\vec{r})$. Therefore $C_n(\vec{r})$ obeys the equation hierarchy

$$\begin{aligned} D\nabla^2 C_0(\vec{r}) &= -\delta(\vec{r} - \vec{r}_0), \\ D\nabla^2 C_1(\vec{r}) &= -C_0(\vec{r}), \\ D\nabla^2 C_2(\vec{r}) &= -2C_1(\vec{r}) \\ &\vdots \end{aligned} \tag{1.6.12}$$

Thus each C_n is the electrostatic "potential" generated by the "charge" distribution C_{n-1}, with $\langle t^n \rangle = n \int_V C_{n-1}(\vec{r})\, d\vec{r}$. This provides all moments of the first-passage time in terms of an associated hierarchy of electrostatic potentials.

1.6.3. Laplacian Formalism

Another useful version of the correspondence between diffusion and electrostatics is based on encoding the initial condition as the spatial argument of an electrostatic potential rather than as an initial condition. This Laplacian approach gives the splitting probability for composite domain boundaries in a natural fashion and also provides *conditional* hitting times, namely, the times to eventually hit a specific subset of the boundary.

1.6.3.1. Splitting Probabilities

For simplicity, we start with a symmetric nearest-neighbor random walk in the finite interval $[x_-, x_+]$ and then take the continuum limit after developing the formalism. We define $\mathcal{E}_-(x)$ as the probability for a particle, which starts at x, to eventually hit x_- *without* hitting x_+. The generalization to higher dimensions and to more general boundaries follows by similar reasoning. Pictorially, we obtain the eventual hitting probability $\mathcal{E}_-(x)$ by summing the probabilities for all paths that start at x and reach x_- without touching x_+ (Fig. 1.4). A parallel statement holds for $\mathcal{E}_+(x)$. Thus

$$\mathcal{E}_\pm(x) = \sum_{P_\pm} \mathcal{P}_{P_\pm}(x), \tag{1.6.13}$$

where $\mathcal{P}_{P_\pm}(x)$ denotes the probability of a path from x to $x_\pm$ that avoids $x_\mp$. As illustrated in Fig. 1.4, the sum over all such restricted paths can be decomposed into the outcome after one step and the sum over all path remainders from the

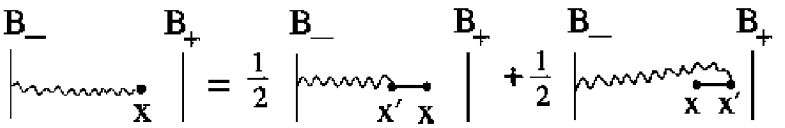


Fig. 1.4. Decomposition of random-walk paths from x to the absorbing subset B_- (the point x_-) into the outcome after one step and the remainder from x' to B_-. The factors $1/2$ account for the probabilities associated with the first step of the decomposed paths.

intermediate point x' to $x_\pm$. This gives

$$\begin{aligned}\mathcal{E}_\pm(x) &= \sum_{p_\pm}\left[\frac{1}{2}\mathcal{P}_{p_\pm}(x+\delta x)+\frac{1}{2}\mathcal{P}_{p_\pm}(x-\delta x)\right]\\ &= \frac{1}{2}[\mathcal{E}_\pm(x+\delta x)+\mathcal{E}_\pm(x-\delta x)].\end{aligned} \tag{1.6.14}$$

By a simple rearrangement, this is equivalent to

$$\Delta^{(2)}\mathcal{E}_\pm(x)=0, \tag{1.6.15}$$

where $\Delta^{(2)}$ is the discrete second-difference operator, which is defined by $\Delta^{(2)}f(x)=f(x-\delta x)-2f(x)+f(x+\delta x)$. Note the opposite sense of this recursion formula compared with master equation Eq. (1.3.1) for the probability distribution. Here $\mathcal{E}\pm(x)$ is expressed in terms of *output from* x, whereas in the master equation, the occupation probability at x is expressed in terms of *input to* x.

The basic Laplace equation (1.6.15) is subject to the boundary conditions $\mathcal{E}_-(x_-)=1, \mathcal{E}_-(x_+)=0$, and correspondingly $\mathcal{E}_+(x_-)=0, \mathcal{E}_+(x_+)=1$. In the continuum limit, Eq. (1.6.15) reduces to the one-dimensional Laplace equation $\mathcal{E}''_\pm(x)=0$. For isotropic diffusion in d spatial dimensions, the corresponding equation is

$$\nabla^2\mathcal{E}_\pm(\vec{r})=0, \tag{1.6.16}$$

subject to the boundary conditions $\mathcal{E}_-(\vec{r}_-)=1$ and $\mathcal{E}_-(\vec{r}_+)=0$; that is, $\mathcal{E}_-=1$ on the exit subset of the absorbing boundary and $\mathcal{E}_-=0$ on the complement of this boundary. These conditions are interchanged for $\mathcal{E}_+$.

The functions $\mathcal{E}_\pm$ are *harmonic* because $\mathcal{E}_\pm(x)$ equals the average of $\mathcal{E}_\pm$ at neighboring points [Eq. (1.6.14)]; that is, $\mathcal{E}_\pm$ is in "harmony" with its local environment. This is a basic feature of solutions to the Laplace equation. Because $\mathcal{E}_\pm$ satisfies the Laplace equation, we can transcribe well-known results from electrostatics to less familiar, but corresponding, first-passage properties. This approach will be applied repeatedly in later chapters.

We can easily extend the Laplacian formalism to a general random-walk process in which the probability of hopping from $\vec{r}$ to $\vec{r}\,'$ in a single step is

$p_{\vec{r}\to\vec{r}'}$. The appropriate generalization of Eq. (1.6.14) is

$$\mathcal{E}_{\pm}(\vec{r}) = \sum_{\vec{r}'} p_{\vec{r}\to\vec{r}'}\mathcal{E}_{\pm}(\vec{r}'), \tag{1.6.17}$$

which, in the continuum limit, reduces to

$$D(\vec{r})\nabla^2\mathcal{E}_{\pm}(\vec{r}) + \vec{v}(\vec{r})\cdot\vec{\nabla}\mathcal{E}_{\pm}(\vec{r}) = 0, \tag{1.6.18}$$

where the local diffusion coefficient $D(\vec{r})$ is just the mean-square displacement and the local velocity $\vec{v}(\vec{r})$ is the mean displacement after a single step when starting from $\vec{r}$ in this hopping process. The existence of the continuum limit requires that the range of the hopping is finite. This equation should be solved subject again to the boundary condition of $\mathcal{E}_{\pm} = 1$ on the exit boundary and $\mathcal{E}_{\pm} = 0$ on the complement of the exit.

In summary, the hitting, or exit, probability coincides with the electrostatic potential when the boundary conditions of the diffusive and the electrostatic systems are the same. This statement applies for both continuum diffusion and the discrete random walk. This approach can be extended in an obvious way to more general hopping processes with both a spatially varying bias and diffusion coefficient. The consequences of this simple equivalence are powerful. As an example, consider a diffusing particle that is initially at radius r_0 exterior to a sphere of radius a centered at the origin in d dimensions. By the electrostatic formalism, the probability that this particle eventually hits the sphere is simply the electrostatic potential at r_0, $\mathcal{E}_{-}(r_0) = (a/r_0)^{d-2}$! Conversely, if a diffusing particle starts in the interior of a bounded domain, it is physically obvious that the boundary is eventually reached. This means that $\mathcal{E}(\vec{r}) = 1$ for any interior point. This also follows from the fact that $\nabla^2\mathcal{E}(\vec{r}) = 0$ within the domain, subject to the boundary condition $\mathcal{E}(\vec{r}) = 1$ on the boundary. The solution is clearly $\mathcal{E}(\vec{r}) = 1$ for any interior point. This corresponds to the well-known fact that the electrostatic potentisl in the interior of a conductor is constant, or equivalently, the electric field is zero.

1.6.3.2. Unconditional and Conditional Mean First-Passage Times

We now extend the Laplacian approach to determine the mean exit time from a domain with composite boundaries. Here we distinguish between the *unconditional* mean exit time, namely, the time for a particle to reach any point on an absorbing boundary B, and the *conditional* mean exit time, namely, the time for a particle to reach a specified subset of the absorbing boundary B_- *without* touching the complement boundary $B_+ = B - B_-$. This conditional exit time is closely related to the splitting probability of Subsection 1.6.3.1.

We again treat a symmetric random walk on the finite interval $[x_-, x_+]$; the generalization to higher dimensions and to general hopping processes is straightforward. Let the time increment between successive steps be δt, and let $t(x)$ denote the mean time to exit at *either* boundary component when a particle starts at x. This quantity is simply the time for each exit path times the probability of the path, averaged over all particle trajectories. This leads to the analog of Eq. (1.6.13):

$$t(x) = \sum_p \mathcal{P}_p(x) t_p(x), \tag{1.6.19}$$

where $t_p(x)$ is the exit time of a specific path to the boundary that starts at x.

In analogy with Eq. (1.6.14), this mean exit time obeys the recursion formula

$$t(x) = \frac{1}{2}\left\{[t(x+\delta x)+\delta t] + [t(x-\delta x)+\delta t]\right\}, \tag{1.6.20}$$

with the boundary conditions $t(x_-) = t(x_+) = 0$, which correspond to the exit time being equal to zero if the particle starts at the boundary. This recursion relation expresses the mean exit time starting at x in terms of the outcome one step in the future, for which the initial walk can be viewed as restarting at either $x + \delta x$ or at $x - \delta x$, each with probability $1/2$, but also with the time incremented by δt. In the continuum limit, the Taylor expansion of this recursion formula to lowest nonvanishing order yields the Poisson equation $Dt''(x) = -1$. For diffusion in a d-dimensional domain with absorption on the boundary B, the corresponding Poisson equation for the exit time is

$$D\nabla^2 t(\vec{r}) = -1, \tag{1.6.21}$$

subject to the boundary condition $t(\vec{r}) = 0$ for $\vec{r} \in B$. This Poisson is often termed the *adjoint equation* for the mean exit, or mean first-passage, time.

These results can be extended to a general short-range hopping process with single-step hopping probability $p_{\vec{r}\to\vec{r}'}$. In this case, the analog of Eq. (1.6.20) is

$$t(\vec{r}') = \sum_{\vec{r}'} p_{\vec{r}\to\vec{r}'}[t(\vec{r}') + \delta t], \tag{1.6.22}$$

which in the continuum limit, becomes the Poisson-like equation

$$D\nabla^2 t(\vec{r}) + \vec{v}(\vec{r}) \cdot \vec{\nabla} t(\vec{r}) = -1. \tag{1.6.23}$$

Note, in particular, that the determination of the mean exit time has been recast as a time-independent electrostatic problem. As we shall see in the next chapters, this device greatly simplifies the computation of the mean exit times and also provides useful physical insights.

Finally, we may extend this electrostatic formalism to the conditional exit times in which we discriminate the exit time by which part of the boundary is reached. Thus let $t_-(x)$ be the conditional mean exit time for a random walk that starts at x and exits at B_- without hitting B_+. Similarly let $t_+(x)$ be the conditional mean exit time for a random walk that starts at x and exits at B_+ without hitting B_-. By its definition, $t_-(x)$ can be written as

$$t_-(x) = \frac{\sum_{p_-} \mathcal{P}_p\ (x)\ t_{p_-}(x)}{\sum_{p_-} \mathcal{P}_{p_-}(x)} = \frac{\sum_{p_-} \mathcal{P}_{p_-}(x)\ t_{p_-}(x)}{\mathcal{E}_-(x)}, \qquad (1.6.24)$$

where the sum over paths p_- denotes only the allowed paths that start at x and reach B_- without touching B_+. By decomposing each path as the outcome after one step and its remainder, and then applying Eq. (1.6.14), we may write

$$\begin{aligned}
\mathcal{E}_-(x)t_-(x) &= \sum_{p_-} \frac{1}{2}[\mathcal{P}_{p_-}(x-\delta x)(t_{p_-}(x-\delta x)+\delta t) \\
&\qquad + \mathcal{P}_{p_-}(x+\delta x)(t_{p_-}(x+\delta x)+\delta t)] \\
&= \delta t\, \mathcal{E}_-(x) + \frac{1}{2}[\mathcal{E}_-(x-\delta x)t_-(x-\delta x) \\
&\qquad + \mathcal{E}_-(x+\delta x)t_-(x+\delta x)] \\
&\approx \delta t\, \mathcal{E}_-(x) + \left[\mathcal{E}_-(x)t_-(x) + \frac{\delta x^2}{2}\frac{\partial^2 \mathcal{E}_-(x)t_-(x)}{\partial x^2}\right]. \qquad (1.6.25)
\end{aligned}$$

In the continuum limit, this leads to a Poisson equation for the conditional mean first-passage time (now written for general spatial dimension)

$$D\nabla^2[\mathcal{E}_-(\vec{r})t_-(\vec{r})] = -\mathcal{E}_-(\vec{r}), \qquad (1.6.26)$$

with $D = 2(\delta r)^2/2\delta t$ and subject to the boundary conditions $\mathcal{E}_-(\vec{r})t_-(\vec{r}) = 0$ both on B_- (where t_- vanishes) and on B_+ (where $\mathcal{E}_-$ vanishes). The governing equations and boundary conditions for $t_+(\vec{r})$ are entirely analogous. Finally, if there is a bias in the hopping process, then Eq. (1.6.26) is generalized to

$$D\nabla^2[\mathcal{E}_\pm(\vec{r})t_\pm(\vec{r})] + \vec{v}(\vec{r}) \cdot \vec{\nabla}[\mathcal{E}_\pm(\vec{r})t_\pm(\vec{r})] = -\mathcal{E}_\pm(\vec{r}). \qquad (1.6.27)$$

With this formalism, we can obtain eventual hitting probabilities and mean hitting times (both unconditional and conditional) by solving time-independent electrostatic boundary-value problems. Thus this electrostatic connection will allow us to obtain subtle conditional first-passage properties in a relatively simple manner.

1.7. Random Walks and Resistor Networks

1.7.1. Introduction

In parallel with the connection between diffusive first-passage properties and the Laplace and the Poisson equations of electrostatics, there is a deep relation between first-passage properties of random walks and the discrete analog of electrostatics. The latter is naturally expressed as the current-carrying properties of a suitably defined resistor network. This is the basis of an appealing mapping between the first-passage characteristics of a random walk on a particular graph and the current-carrying properties of a resistor network whose elements consist of the same graph. We shall show that the voltages at each site and the overall network resistance are directly and simply related to the exit probabilities of a corresponding random walk. Our discussion closely follows that given in Doyle and Snell (1984).

1.7.2. The Basic Relation

To develop the resistor network connection, consider a discrete random walk on a finite lattice graph with hopping between nearest-neighbor sites (see Fig. 1.5). We divide the boundary points into two classes, B_+ and B_-. As usual, we are interested in the exit probabilities to B_+ and to B_- as functions of the initial position x of the random walk. As shown in Section 1.6, these exit probabilities, $\mathcal{E}_+(x)$, and $\mathcal{E}_-(x)$, respectively, are governed by the discrete Laplace equation $\Delta^{(2)}\mathcal{E}_\pm(x) = 0$, subject to the boundary conditions $\mathcal{E}_+ = 1$ on B_+ and $\mathcal{E}_+ = 0$ on B_- and vice versa for $\mathcal{E}_-$.

This Laplace equation has a simple resistor network interpretation. The basic connection is that if all the lattice bonds are viewed as resistors (not necessarily identical), then Kirchhoff's laws for steady current flow in the

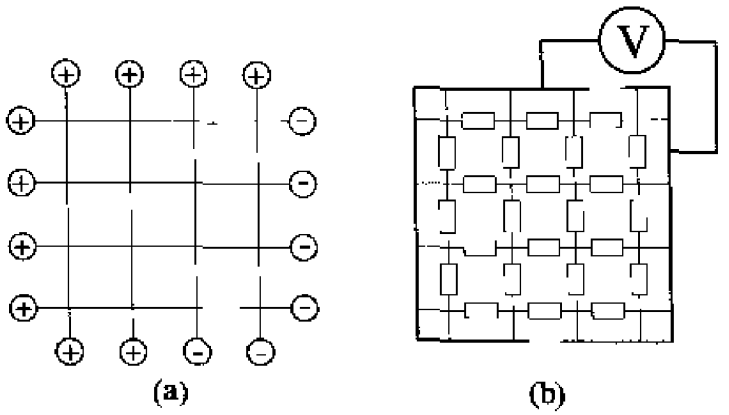


Fig. 1.5. (a) A lattice graph with boundary sites B_+ or B_-. (b) Corresponding resistor network in which each bond (with rectangle) is a 1-Ω resistor. The sites in B_+ are all fixed at potential $V = 1$, and sites in B_- are all grounded.

network are identical to the discrete Laplace equation for $\mathcal{E}$. Suppose that the boundary sites in B_+ are fixed at unit potential while the sites in B_- are grounded. The net current at each interior site i of the network must be zero, as there is current input and output only at the boundary. This current conservation condition is

$$\sum_j g_{ij}(V_i - V_j) = 0. \tag{1.7.1}$$

where g_{ij} is the conductance of the bond between sites i and j, V_i is the voltage at site i, and the sum rons over the nearest neighbors j of site i. Solving for V_i gives

$$V_i = \frac{\sum_j g_{ij} V_j}{\sum_j g_{ij}} \to \frac{1}{4}\sum_j V_j, \tag{1.7.2}$$

where the last step applies for a homogeneous network. Thus, in the steady state, the voltage at each interior site equals the weighted average of the voltages at the neighboring sites; that is, V_i is a harmonic function with respect to the weight function g_{ij}. The voltage must also satisfy the boundary conditions $V = 1$ for sites in B_+ and $V = 0$ for sites in B_-.

We can also give a random-walk interpretation for the process defined by Eq. (1.7.2). Consider a lattice random walk in which the probability of hopping from site i to site j is $P_{ij} = g_{ij}/\sum_j g_{ij}$. Then the probability that this walk eventually reaches B_+ without first reaching B_- is just given by $\mathcal{E}_+(i) = \sum_{p_+} \mathcal{P}_{p_+}(i)$ [see Eqs. (1.6.13)–(1.6.15)]. Because both V_i and $\mathcal{E}_+(i)$ are harmonic functions that satisfy the same boundary conditions, these two functions are identical. Thus we find the basic relation between random walks and resistor networks:

- Let the boundary sets B_+ and B_- in a resistor network be fixed at voltages 1 and 0 respectively, with g_{ij} the conductance of the bond between sites i and j. Then the voltage at any interior site i is the same as the probability for a random walk that starts at i to reach B_+ before reaching B_- when the hopping probability from i to j is $P_{ij} = g_{ij}/\sum_j g_{ij}$.

1.7.3. Escape Probability, Resistance, and Pólya's Theorem

An important extension of this relation between escape probability and site voltages is to infinite networks. This provides a simple connection between the recurrence/transience transition of random walks on a given network and the electrical resistance of this same network. Suppose that the voltage V at the boundary sites B_+ is set to one. Then the total current entering the network

is given by

$$I = \sum_j (V - V_j) g_{+j}$$
$$= \sum_j (1 - V_j) P_{+j} \sum_j g_{+j}. \tag{1.7.3}$$

Here g_{+j} is the conductance between the positive terminal of the voltage source and the neighboring sites j and $P_{+j} = g_{+j} / \sum_j g_{+j}$. Because the voltage V_j also equals the probability for the corresponding random walk to reach B_+ without reaching B_-, the term $V_j P_{+j}$ is just the probability that a random walk starts at B_+, makes a single step to the sites j (with hopping probabilities P_{+j}), and then returns to B_+ without reaching B_-. We therefore deduce that

$$I = \sum_j g_{+j} \sum_j (1 - V_j) P_{+j}$$
$$= \sum_j g_{+j} \times (1 - \text{return probability})$$
$$= \sum_j g_{+j} \times \text{escape probability}. \tag{1.7.4}$$

Here "escape" means reaching the opposite terminal of the voltage source without returning to the starting point.

On the other hand, the input current and the voltage drop across the network are simply related to the conductance G between the two boundary sets by $I = GV = G$. From this and Eq. (1.7.4) we obtain the fundamental result:

$$\text{escape probability} \equiv P_{\text{escape}} = \frac{G}{\sum_j g_{+j}}. \tag{1.7.5}$$

Perhaps the most interesting situation is when a current I is injected at a single point of an infinite network with outflow at infinity (see Fig. 1.6). Then the probability for a random walk that starts at this input point to escape, that is, never return to its starting point, is simply proportional to the network conductance G. It is amazing that a subtle feature of random walks is directly related to currents and voltages in a resistor network!

One appeal of this connection is that network conductances can be computed easily. In one dimension, the conductance of an infinitely long chain of identical resistors is clearly zero. Thus $P_{\text{escape}} = 0$ or, equivalently, $P_{\text{return}} = 1$; that is, a random walk in one dimension is recurrent. In higher dimensions,

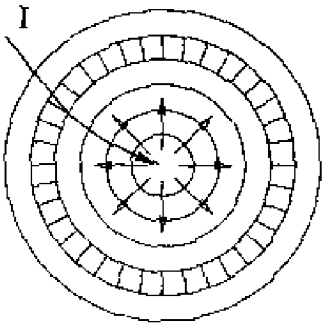


Fig. 1.6. Decomposition of a conducting medium into concentric shells, each of which consists of fixed-conductance blocks. A current I is injected at the origin and flows radially outward through the medium.

the conductance between one point and infinity in an infinite resistor lattice is a beautiful and more demanding problem that has inspired many physicists [see e.g., van der Pol & Bremmer (1955), see also Atkinson & van Steenwijk (1999) and Cserti (2000) for more recent pedagogical accounts]. However, for merely determining the recurrence or transience of a random walk, a crude physical estimate suffices. The basic idea of this estimate is to replace the discrete lattice with a continuum medium of constant conductivity. We then compute the conductance of the infinite system by further decomposing the medium into a series of concentric shells of fixed thickness dr. A shell at radius r can be regarded as a parallel array of r^{d-1} volume elements, each of which has a fixed conductance. The conductance of one such a shell is then simply proportional to its surface area, and the overall resistance is the sum of the shell resistance. This gives

$$R \sim \int^{\infty} R_{\rm shell}(r)\, dr \sim \int^{\infty} \frac{dr}{r^{d-1}} \tag{1.7.6}$$

$$= \begin{cases} \infty & \text{for } d \leq 2 \\ \left(P_{\rm escape} \sum_j g_{+j}\right)^{-1} & \text{for } d > 2 \end{cases} \tag{1.7.7}$$

This provides a remarkably easy solution to the recurrence/transience transition of random walks. For $d > 2$, the conductance between a single point and infinity in an infinite homogeneous resistor network is nonzero and is simply related to the random-walk escape probability. For $d \leq 2$, the conductance to infinity is zero, essentially because there are an insufficient number of independent paths from the origin to infinity. Correspondingly, the escape probability is zero and the random walk is recurrent. The case $d = 2$ is more

delicate because the integral in expression (1.7.6) diverges only logarithmically at the upper limit. Nevertheless, the conductance to infinity slowly goes to zero as the radius of the network diverges and the corresponding escape probability is still zero.

1.8. Epilogue

The approaches outlined in this chapter provide the tools to determine where a diffusing particle gets trapped on, or exits from, an absorbing boundary and how long it takes for this event to occur. Often we can determine these properties most elegantly by mapping the diffusion problem onto a corresponding electrostatic problem or onto a resistor network problem (in the case of random walks). These mappings have powerful implications yet are generally easy to apply. This use of the analogy to electrostatics underlies much of the mathematical literature on first passage [see, e.g., Dynkin & Yushkevich (1969), Spitzer (1976), and Salminen & Borodin (1996)].

Another related message that will become even more apparent in the next chapter is that it is invariably much easier to deal with continuum diffusion and its corresponding electrostatics, rather than with discrete random walks. Although the generating function formalism is an elegant and powerful way to treat the dynamics of random walks and their associated first-passage properties [Montroll (1965), Montroll & Weiss (1965), and Weiss & Rubin (1983)], the corresponding properties are much easier to treat in the continuum-diffusion approximation. Thus we will concentrate primarily on diffusion and return to discrete random walks only for pedagogical completeness or when random walks provide the most appropriate description of a particular system. Our main goal in the following chapters is to elucidate the first-passage properties of diffusion and its physical implications for a variety of physically relevant systems, both by direct methods and by exploiting the connections with electrostatics.