3 SEMI-INFINITE SYSTEM

3.1 The Basic Dichotomy

A natural counterpart to the finite interval is the first-passage properties of the semi-infinite interval \((0, \infty)\) with absorption at \(x = 0\). Once again, this is a classical geometry for studying first-passage processes and many of the references mentioned at the outset of Chap. 2 are again pertinent. In particular, the text by Karlin & Taylor (1975) gives a particularly comprehensive discussion about first-passage times in the semi-infinite interval with arbitrary hopping rates between neighboring sites. Once again, however, our focus is on simple diffusion or the nearest-neighbor random walk. For these processes, the possibility of a diffusing particle making arbitrarily large excursions before certain trapping takes place leads to an infinite mean lifetime. On the other hand, the recurrence of diffusion in one dimension means that the particle must eventually return to its starting point. This dichotomy between infinite lifetime and certain trapping leads to a variety of extremely surprising first-passage-related properties both for the semi-infinite interval and the infinite system.

Perhaps the most amazing such property is the arcsine law for the probability of long leads in a symmetric nearest-neighbor random walk in an unbounded domain. Although this law applies to the unrestricted random walk, it is intimately based on the statistics of returns to the origin and thus fits naturally in our discussion of first-passage on the semi-infinite interval. Our natural expectation is that, for a random walk which starts at \(x = 0\), approximately one-half of the total time would be spent on the positive axis and the remaining one-half of the time on the negative axis. Surprisingly, this is the least probable outcome. In fact, the arcsine law tells us that the most probable outcome is that the walk always remains entirely on the positive or on the negative axis.

We will begin by presenting the very appealing image method to solve the first-passage properties in the semi-infinite interval. This approach can be extended easily to treat biased diffusion. We then turn to the discrete random walk and explore some intriguing consequences of the fundamental dichotomy between certain return and infinite return time, such as the arcsine law. We will also treat the role of partial trapping at the origin which leads naturally to a useful correspondence with diffusion in an attenuating medium and also the radiation boundary condition. Finally, we discuss the quasi-static approximation. This is a simple yet powerful approach for understanding diffusion near an absorbing boundary in terms of an effective, nearly time-independent system. This approach provides the simplest way to treat first-passage in higher dimensions, to be presented in Chap. 6.

3.2 Image Method

3.2.1 The Concentration Profile

We determine the first-passage probability to the origin for a diffusing particle which starts at \(x_0 > 0\) subject to the absorbing boundary condition that the concentration \(c(x, t)\) at the origin is zero. The most appealing method of solution is the familiar image method from electrodynamics. In this method, a particle initially at \(x = x_0\) and an image “antiparticle” initially at \(x = -x_0\) which both diffuse freely on \([-\infty, \infty]\) give a
resultant concentration \( c(x, t) \) which obviously satisfies the absorbing boundary condition \( c(0, t) = 0 \). Thus in the half-space \( x > 0 \), the image solution coincides with the concentration of the initial absorbing boundary condition system.

Hence we may write the concentration (or probability distribution) for a diffusing particle on the positive half-line as the sum of a Gaussian and an anti-Gaussian

\[
c(x, t) = \frac{1}{\sqrt{4\pi Dt}} \left[ e^{-\frac{(x-x_0)^2}{4Dt}} - e^{-\frac{(x+x_0)^2}{4Dt}} \right].
\]  

(3.2.1)

In the long-time limit, it is instructive to rewrite this as

\[
c(x, t) \approx \frac{1}{\sqrt{4\pi Dt}} \frac{x_0}{Dt} e^{-\frac{(x^2+x_0^2)}{4Dt}},
\]  

(3.2.2)

which clearly exhibits its short- and large-distance tails. We see that the concentration has a linear dependence on \( x \) near the origin and a Gaussian large-distance tail, as illustrated in Fig. 3.1.

![Fig. 3.1. Concentration profile of a diffusing particle in the absorbing semi-infinite interval (0, ∞) at Dt = 10, with x₀ = 2. Shown are the component Gaussian and image anti-Gaussian (dashed curves) and their superposition in the physical region x > 0 (solid curves).](image)

A crude but useful way to visualize the concentration and to obtain first-passage characteristics quite simply is to replace the constituent Gaussian and anti-Gaussian in the image solution by simpler functions which have the general scaling properties as these Gaussians. Thus we replace the initial Gaussian by a “blip” function centered at \( x_0 \), of width \( \sqrt{D} \) and amplitude \( 1/\sqrt{D} \), and the anti-Gaussian by an “anti-blip” at \( -x_0 \), of width \( \sqrt{D} \) and amplitude \( -1/\sqrt{D} \). Their superposition gives a constant distribution of magnitude \( 1/\sqrt{D} \) which extends from \( \frac{1}{2}\sqrt{D} - x_0 \) to \( \frac{1}{2}\sqrt{D} + x_0 \) (Fig 3.2). From this picture, we immediately infer that the survival probability varies as \( S(t) \approx 2x_0/\sqrt{Dt} \), while the mean displacement of the probability distribution which remains alive recedes from the trap as \( \sqrt{Dt} \). While this use of blip functions provides
a modest simplification for the semi-infinite line, this cartoon-like approach is extremely useful for more complicated geometries, such as diffusion within an absorbing wedge (see Chap. 7).

\[ \frac{\sqrt{Dt}}{2x_0} \]

![Diagram](image)

Fig. 3.2. Superposition (solid) of a blip and anti-blip (dashed) to crudely represent the probability distribution for diffusion on \((0, \infty)\) with an absorber at \(x = 0\).

As a concluding note to this section, it is worth pointing out an amusing extension of the image method. Let us work backward by introducing a suitably-defined image and then determine the locus on which the concentration due to the particle and the image vanishes. This then immediately provides the solution to a corresponding boundary value problem.

To provide a flavor for this method, consider the simple example of a particle which starts at \(x_0\) and an image, with weight \(-w\) \(\neq 1\), which starts at \(-x_0\). The total concentration that is due to these two sources is

\[
c(x, t) = \frac{1}{\sqrt{4\pi Dt}} \left[ e^{-(x-x_0)^2/(4Dt)} - we^{-(x+x_0)^2/(4Dt)} \right],
\]

which clearly vanishes on the locus \(x(t) = \frac{D}{2x_0} \ln w\). Therefore the solution to the diffusion equation in the presence of an absorbing boundary that moves at constant speed \(v\) is given by the sum of a Gaussian and an image anti-Gaussian of amplitude \(w = e^{vx_0/D}\). By being judicious, this approach can be extended to treat a surprisingly wide variety of absorbing boundary geometries (Daniels (1969); Daniels (1982)).

### 3.2.2 First-Passage Properties

#### 3.2.2.1 Isotropic Diffusion

Since the initial condition is normalized, the first-passage probability to the origin at time \(t\) is just the flux to this point. From the exact expression for \(c(x, t)\) in Eq. (3.2.1), we find

\[
F(0, t) = +D \frac{\partial c(x, t)}{\partial x} \bigg|_{x=0} = \frac{x_0}{\sqrt{4\pi Dt^3}} e^{-x_0^2/(4Dt)} \quad t \to \infty.
\]

This distribution is sometimes termed the inverse Gaussian density (see Chikara & Folks (1989) for a general discussion about this distribution). In the long time limit \(\sqrt{Dt} \gg x_0\), for which the diffusion length is much greater than the initial distance to the origin, the first-passage probability reduces to \(F(0, t) \to x_0/t^{3/2}\), as was derived in Chap. 1 by extracting the first-passage probability directly from the underlying probability
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distribution. The existence of this long-time tail means that the mean time for the particle to reach the origin is infinite! That is
\[
\langle t \rangle \equiv \int_0^\infty t F(0, t) \, dt \sim \int_0^\infty t \times t^{-3/2} \, dt = \infty.
\] (3.2.5)
On the other hand, the particle is sure to return to the origin because \( \int_0^\infty F(t) \, dt = 1 \).

Although the mean time to return to the origin is infinite, suitably-defined low-order moments are finite. In general, the \( k \)-th moment is
\[
\langle t^k \rangle = \frac{x_0}{\sqrt{4\pi D}} \int_0^\infty t^{k-3/2} e^{-x_0^2/4Dt} \, dt.
\] (3.2.6)
This integral converges for \( k < 1/2 \), so that moments of order less than 1/2 are finite. By elementary steps, we explicitly find
\[
\langle t^k \rangle = \frac{\Gamma\left(\frac{1}{2} - k\right)}{\sqrt{\pi} \left(\frac{x_0^2}{4D}\right)^k}.
\] (3.2.7)

For \( k < 1/2 \), the units of \( \langle t^k \rangle \) are determined by the time to diffuse a distance \( x_0 \), which is the only natural time scale in the problem. The finiteness of these low-order moments is yet another manifestation of the dichotomy between certain return and infinite return time for one-dimensional diffusion. An application of these results to neuron dynamics will be given in Section 4.2.

From the first-passage probability, the survival probability \( S(t) \) may be found directly through \( S(t) = 1 - \int_0^t F(0, t') \, dt' \), or it may be obtained by integrating the concentration over positive \( x \). The former approach gives
\[
S(t) = 1 - \int_0^t \frac{x_0}{\sqrt{4\pi Dt'^3}} e^{-x_0^2/4Dt'} \, dt',
\] (3.2.8)
and we may evaluate this integral easily by rewriting the integrand in terms of \( u^2 = x_0^2/4Dt' \) to give
\[
S(t) = 1 + \frac{2}{\sqrt{\pi}} \int_{x_0/\sqrt{4Dt}}^\infty e^{-u^2} \, du
\]
\[
= \frac{2}{\sqrt{\pi}} \int_0^{x_0/\sqrt{4Dt}} e^{-u^2} \, du
\]
\[
= \text{erf}(\frac{x_0}{\sqrt{4Dt}}).
\] (3.2.9a)
Alternatively, integrating of the probability distribution over the positive interval gives
\[
S(t) = \int_0^\infty c(x, t) \, dx
\]
\[
= \frac{1}{\sqrt{4\pi Dt}} \left[ \int_0^\infty dx e^{-(x-x_0)^2/4Dt} - \int_0^\infty dx e^{-(x+x_0)^2/4Dt} \right]
\]
\[
= \frac{1}{\sqrt{\pi}} \int_{-x_0/\sqrt{4Dt}}^{\infty} e^{-u^2} \, du - \frac{1}{\sqrt{\pi}} \int_{-\infty}^{-x_0/\sqrt{4Dt}} e^{-u^2} \, du
\]
\[
= \frac{2}{\sqrt{\pi}} \int_0^{x_0/\sqrt{4Dt}} e^{-u^2} \, du
\]
\[
= \text{erf}(\frac{x_0}{\sqrt{4Dt}}).
\] (3.2.9b)

From this result, the survival probability is nearly constant until the diffusion length \( \sqrt{Dt} \) reaches the initial distance to the boundary, \( x_0 \). Subsequently, the particle has the opportunity to reach the origin by diffusion, and trapping becomes significant. For \( \sqrt{Dt} \gg x_0 \), the asymptotic behavior of the error function
Fig. 3.3. Double logarithmic plot of survival probability $S(t)$ versus time for $x_0 = 10$. The survival probability remains close to one for $Dt < x_0^2$ and then decays as $t^{-1/2}$ thereafter.

(Abramowitz & Stegun (1972)) then gives

$$S(t) \sim \frac{x_0}{\sqrt{\pi Dt}}$$

(3.2.10)

As expected by the recurrence of diffusion, the survival probability ultimately decays to zero. The $1/\sqrt{Dt}$ long-time behavior is clearly evident in Fig. 3.3.

Let us re-interpret these properties within the framework of the nervous investor example of Chap. 1. An investor buys a share of stock at $100$ in a market in which the price changes equiprobably by a factor $f = 0.9$ or $f^{-1}$ daily. After one day, the stock price drops to $90$ (one step away from the boundary) and the investor decides to sell out when the initial price is recovered. Unlike our example in Chap. 1, our investor now has infinite fortitude and will not sell until break-even again occurs. That is, the process is now defined on the semi-infinite interval. Thus an average investor must be both patient and willing to accept an arbitrarily large intermediate loss to ensure a sale at the break-even point. After $t$ trading days, a fraction $1 - 1/\sqrt{t}$ of the traders will break even, while the remaining unlucky fraction $1/\sqrt{t}$ of the traders will typically see their stock worth $100 \times f^{\sqrt{t}}$. For example, after 50 days, approximately 14% of the investors are still in the market and the stock price will typically sink to approximately $47$.

It is also useful to study the spatial dependence of the probability distribution. As seen most clearly in Fig. 3.2, the surviving fraction recedes from the origin with a mean displacement $\sqrt{Dt}$ – a particle must move away from the origin to be long lived. This is clearly evident in the mean displacement of the distribution of surviving particles. Following the same steps as those used to compute the survival probability, we find that this displacement is

$$\langle x \rangle = \frac{1}{S(t)} \frac{1}{\sqrt{4\pi Dt}} \int_{0}^{\infty} x \left[ e^{-(x-x_0)^2/4Dt} - e^{-(x+x_0)^2/4Dt} \right] dx$$

$$= \frac{1}{S(t)} \frac{1}{\sqrt{\pi}} \int_{-x_0/\sqrt{4Dt}}^{\infty} (u \sqrt{4Dt} + x_0)e^{-u^2} du$$
Within a scaling approach, this fact alone is sufficient to give the solution to the convection-diffusion equation in the domain. Let the dependence on $x$ consist of an image contribution which moves in the opposite direction compared with that of the initial particle. Thus we anticipate that the function $f(x)$ may be expressed as

$$
\langle x \rangle = x_0 f \left( \frac{Dt}{x_0^2} \right).
$$

Here the scaling function $f(u)$ must approach a constant for small $u$, so that we recover $x(t) \to x_0$ as $t \to 0$. On the other hand, at long times $Dt \gg x_0^2$, the initial position of the particle should become irrelevant. This occurs only if $f(u) \propto u^{1/2}$ for large $u$. By using this form for $f(u)$, we see that $\langle x \rangle$ grows as $\sqrt{Dt}$ and that the dependence on $x_0$ also disappears in the long-time limit. This reproduces the long-time behavior given in Eq. (3.2.11).

### 3.2.2.2 Biased Diffusion

A nice feature of the image method is that it can be adapted in a simple but elegant manner to biased diffusion. Naively, we might anticipate that if the particle has a drift velocity $v$, the image particle should move with velocity $-v$. However, because of this opposite velocity, such an image contribution would not satisfy the initial convection-diffusion equation in the domain $x > 0$. The correct solution must therefore consist of an image contribution which moves in the same direction as that of the original particle to satisfy the equation of motion. By inspection, the solution is

$$
c(x, t) = \frac{1}{\sqrt{4\pi Dt}} \left[ e^{-(x-x_0-vt)^2/4Dt} - e^{-vx_0/D} e^{-(x+x_0-vt)^2/4Dt} \right],
$$

where the factor $e^{-vx_0/D}$ ensures that $c(x=0, t) = 0$. Notice that by transforming to a reference frame which moves at velocity $v$, we map to the problem of a particle and a static image of magnitude $e^{-vx_0/D}$, together with an absorbing boundary which moves with velocity $-v$. This is the just the problem already solved in Eq. (3.2.3)!

Another basic feature of the image solution is that it is manifestly positive for all $x > 0$, as we can see by rewriting $c(x, t)$ as

$$
c(x, t) = \frac{1}{\sqrt{4\pi Dt}} e^{-(x-x_0-vt)^2/4Dt} \left[ 1 - e^{-vx_0/Dt} \right].
$$

Notice also that Eq. (3.2.12) can be rewritten as

$$
c(x, t) = \frac{1}{\sqrt{4\pi Dt}} \left[ e^{-(x-x_0-vt)^2/4Dt} - e^{vx/D} e^{-(x+x_0+vt)^2/4Dt} \right].
$$

In this representation, the image appears to move in the opposite direction compared with that of the initial
particle. However, the image contribution contains a position-dependent prefactor which decays sufficiently rapidly for large negative \( x \) that the true motion of this image contribution is actually in the same direction as that of the original particle.

From the concentration profile, we determine the first-passage probability either by computing the flux to the origin, \( \nu c - Dc' \big|_{x=0} \), or by Taylor expanding Eq. (3.2.12) in a power series in \( x \) and identifying the linear term with the first-passage probability. Either approach leads to the simple result

\[
F(0, t) = \frac{x_0}{\sqrt{4\pi D t}} e^{-\left(x_0 + vt\right)^2/4Dt}.
\]  

(3.2.13)

As we might expect, this first-passage probability asymptotically decays exponentially in time because of the bias. For negative bias, the particle is very likely to be trapped quickly, while for positive bias the particle very likely escapes to \( +\infty \). In either case the first-passage probability should become vanishingly small in the long-time limit.

From the first-passage probability, the survival probability is

\[
S(t) = 1 - \int_0^t F(0, t') dt',
\]

(3.2.14)

Using again the substitution \( u^2 = x_0^2 / 4Dt \) and the Péclet number \( Pe = \nu x_0 / 2D \), we find that the survival probability is

\[
S(t) = 1 - \frac{2}{\sqrt{\pi}} e^{-Pe} \int_{x_0 / \sqrt{4Dt}}^{\infty} e^{-u^2 - Pe^2 / 4a^2} du
\]

\[
= 1 - \frac{1}{2} e^{-Pe} \left[ 1 - \operatorname{erf} \left( \frac{x_0}{2\sqrt{4Dt}} \right) \right] + e^{-Pe} \left[ 1 - \operatorname{erf} \left( \frac{x_0}{2\sqrt{4Dt}} - \frac{Pe}{2} \frac{\sqrt{4Dt}}{x_0} \right) \right]
\]

\[
\sim 1 - \frac{1}{2} e^{-Pe - |Pe|} \left[ 2 - \operatorname{erfc} \left( \frac{|Pe|}{2} \frac{\sqrt{4Dt}}{x_0} \right) \right], \quad t \to \infty.
\]

(3.2.15)

This last expression has two different behaviors depending on whether the velocity is positive or negative. Using the asymptotic properties of the error function, we find

\[
S(t) \sim \begin{cases} 
1 - e^{-2Pe} = 1 - e^{-\nu x_0 / D}, & \text{for } Pe > 0 \\
\left( \frac{x_0}{\sqrt{4Dt}} \right)^3 \frac{1}{\sqrt{4\pi Pe^2}} e^{-\frac{D}{2}t / x_0^2} = \sqrt{\frac{4 x_0 \sqrt{D} t}{\pi (vt)^2}} e^{-v^2 t / 4D} & \text{for } Pe \leq 0
\end{cases}.
\]  

(3.2.16)

From this result, the probability for the particle to be eventually trapped as a function of its starting location, \( \mathcal{E}(x_0) \), is simply

\[
\mathcal{E}(x_0) = \begin{cases} 
1 - e^{-\nu x_0 / D}, & \text{for } v > 0; \\
1, & \text{for } v \leq 0
\end{cases}.
\]  

(3.2.17)

Thus for zero or negative bias, a diffusing particle is recurrent, while for a positive bias, no matter how small, a diffusing particle is transient. This is a basic extension of the recurrence/transience transition to biased diffusion. Notice, finally, that this last result can be obtained more simply from the Laplacian formalism of Chap. 1. For biased diffusion, \( \mathcal{E}(x) \) satisfies (see Eq. (1.6.18))

\[
D\mathcal{E}'' + \nu \mathcal{E}' = 0,
\]

subject to the boundary conditions \( \mathcal{E}(0) = 1 \) and \( \mathcal{E}(\infty) = 0 \). The first condition corresponds to certain
trapping if the particle starts at the origin, and the second merely states that there is zero trapping probability if the particle starts infinitely far away. The solution to this equation is simply Eq. (3.2.17).

3.2.2.3 Long-Range and Generalized Hopping Processes

For long-range hopping, there is a remarkable and not-so-well-known theorem (to physicists at least), which is due to Sparre Andersen, about first passage in the semi-infinite interval (Sparre Andersen (1953), see also Feller (1968); Spitzer (1976)). For concreteness, consider a discrete time random walk which starts at \( x_0 > 0 \) with each step chosen from a symmetric, continuous, but otherwise arbitrary distribution. Then the probability that the random walk first crosses the origin and hits a point on the negative axis at the \( n^{th} \) step, \( \mathcal{F}(n) \), asymptotically decays as \( n^{-3/2} \), just as in the symmetric nearest-neighbor random walk!

The precise statement of the Sparre Andersen theorem is the following: Let \( \mathcal{F}(z) = \sum_{n=1}^{\infty} \mathcal{F}(n) z^n \) be the generating function for the first-passage probability. Then for a particle which begins at \( x = 0^+ \),

\[
\mathcal{F}(z) = 1 - \sqrt{1 - z}, \quad \text{long-range hopping.}
\]

To put this in context, for the symmetric nearest-neighbor random walk, the generating function for the first-passage probability has the nearly identical form (Eq. (1.5.5))

\[
\mathcal{F}(z) = 1 - 1 - z^2, \quad \text{nearest-neighbor hopping.}
\]

Clearly these two functions have identical singular behaviors as \( z \to 1 \), so that their respectively large-\( n \) properties are also the same. It is especially intriguing that even for a broad distribution of step lengths in which the mean step length is divergent, the probability of first crossing the origin at the \( n^{th} \) still decays as \( n^{-3/2} \).

This theorem can be easily applied to more general situations. One instructive example is the first-passage probability of a long-range hopping process where the time for each step equals the step distance. Suppose that the step lengths \( \ell \) are drawn from a continuous, symmetric distribution \( f(\ell) \sim \ell^{-(1+\mu)} \) for large \( \ell \), with \( 0 < \mu < 1 \) so that the mean step length diverges and the distribution is normalizable. For a particle which starts at \( x_0 > 0 \), we can now find the probability that the particle first hits the region \( x < 0 \) at time \( t \) by the Sparre Andersen theorem.

After a time \( t \), we may determine the number of steps in the walk by first computing the mean step length in a walk of total duration \( t \). This length is

\[
\int_0^t \ell f(\ell) \, d\ell \propto t^{1-\mu}.
\]

For this finite-duration walk, the mean step length \( t^{1-\mu} \) times the number of steps \( n(t) \) must clearly equal the total elapsed time \( t \); thus \( n(t) \sim t^\mu \). Now we may transform from the first-passage probability as a function of \( n \) to the first-passage probability as a function of \( t \) by means of

\[
\mathcal{F}(t) = \mathcal{F}(n) \frac{dn}{dt} \propto n^{-3/2} t^{\mu-1} \sim t^{-1+(1+\mu)/2}. \quad (3.2.18)
\]

As an example, consider the following diffusion process in the two-dimensional half-space \((x > 0, y)\) with absorption when \( x = 0 \) is reached (Redner & Krapivsky (1996)). In addition to diffusion, there is a bias \( v_x(y) = \text{sign}(y) \). Thus the bias is directed toward the “cliff” for \( y < 0 \) and away from it for \( y > 0 \) (Fig. 3.4). How does this “schizophrenic” bias (with mean longitudinal velocity zero) affect the particle survival probability? The key to understanding this problem is to notice that successive returns of the vertical displacement to \( y = 0 \) are governed by the one-dimensional first-passage probability. Therefore the displacement \( \ell \) of the particle in the \( x \)-direction between each return has a power-law tail \( \ell^{-3/2} \), corresponding to the case \( \mu = 1/2 \) in the previous two paragraphs. Substituting this into Eq. (3.2.18), we conclude that the first-passage probability decays as \( t^{-5/4} \), corresponding to a survival probability which asymptotically decays as \( t^{-1/4} \). Consequently this bias leads to an increased survival probability compared to pure diffusion.

Amusingly, this \( t^{-5/4} \) decay of the first-passage probability for a Brownian particle in the half-space
3.2 Image Method

![Diagram of a diffusing particle trajectory](image.png)

Fig. 3.4. A typical trajectory of a diffusing particle in the flow field \( v_x(y) = \text{sign}(y) \). The distribution of distances \( \ell \) between successive crossings of \( y = 0 \), \( \ell = x_n - x_{n-1} \), has a \( \ell^{-3/2} \) tail.

geometry appears to be relatively ubiquitous. This same decay occurs for free acceleration in the \( x \)-direction (Sinai (1992); Burkhardt (2000)), for unidirectional general shear flows of the form \( v_x(y) = -v_x(-y) \) (Redner \& Krapivsky (1996)), as well as for a Brownian particle which is subject to a random velocity field in the \( x \)-direction, in which \( v_x(y) \) is a random zero-mean function of \( y \) (Redner (1997)). Perhaps there is a deep relation which connects these apparently disparate systems.

3.2.2.4 Semi-Infinite Slab

We can easily extend our results for the semi-infinite interval to a semi-infinite slab in arbitrary spatial dimension. While the time dependence of the first-passage probability remains the same as in one dimension, we may also study where the particle hits the boundary. Consider the semi-infinite \( d \)-dimensional slab where the last co-ordinate \( x_d \) is restricted to positive values by the absorbing boundary condition at \( x_d = 0 \). A diffusing particle starts at \( \vec{h}_0 = (0, 0, \ldots, 0, h_0) \). What is the probability that the particle eventually hits at some point on the \( (d - 1) \)-dimensional absorbing plane \( x_d = 0 \)?

We may answer this question easily by the image method. First, consider the case of two dimensions. For a particle which starts at \( (0, y_0) \) with the line \( y = 0 \) absorbing, the time-dependent concentration is

\[
 c(x, y, t) = \frac{1}{4\pi Dt} \left[ e^{-(x^2+(y-y_0)^2)/4Dt} - e^{-(x^2+(y+y_0)^2)/4Dt} \right].
\]  

The first-passage probability to any point along the absorbing line at time \( t \) is then the magnitude of the diffusive flux at \( (x, 0) \),

\[
 j(x, 0, t) = D \left. \frac{\partial c(x, y, t)}{\partial y} \right|_{y=0} = \frac{y_0}{4\pi Dt} e^{-(x^2+y_0^2)/4Dt}.
\]

Finally, the probability that the particle eventually hits \( (x, 0) \), \( \mathcal{E}(x; 0, y_0) \), is the integral of the first-passage probability at \( (x, 0) \) over all time,

\[
 \mathcal{E}(x; 0, y_0) = \int_0^\infty j(x, 0, t) \, dt.
\]
We may evaluate this integral easily by changing variables to \( u = (x^2 + y_0^2)/4Dt \) to obtain the Cauchy distribution for the hitting probability,

\[
\mathcal{E}(x; 0, y_0) = \frac{1}{\pi x^2 + y_0^2}.
\] (3.2.21)

Because of the \( x^{-2} \) decay of this distribution for large \( x \), the mean position of a particle which hits the line, namely, \( \langle x \rangle = \int_0^\infty x \mathcal{E}(x; 0, y_0) \, dx \), is infinite.

For general spatial dimension, the time-dependent concentration is

\[
c(\vec{x}, t) = \frac{1}{(4\pi Dt)^{d/2}} \left[ e^{-(\vec{x}_\perp^2 + (x_d - h_0)^2)/4Dt} - e^{-(\vec{x}_\perp^2 + (x_d + h_0)^2)/4Dt} \right],
\] (3.2.22)

where \( \vec{x}_\perp = x_1^2 + x_2^2 + \ldots + x_{d-1}^2 \). From this, the first-passage probability to a point on the absorbing hyperplane is

\[
j(\vec{x}_\perp, t) = \frac{1}{(4\pi Dt)^{d/2}} \frac{h_0}{t} e^{-(\vec{x}_\perp^2 + h_0^2)/4Dt}.
\] (3.2.23)

Integrating over all time and using the same variable change as in two dimensions, we find that the probability of eventually hitting \( \vec{x}_\perp \) is simply

\[
\mathcal{E}(\vec{x}_\perp; \vec{h}_0) = \frac{h_0}{\pi^{d/2} (\vec{x}_\perp^2 + h_0^2)^{d/2}}.
\] (3.2.24)

In greater than two dimensions, the mean lateral position of the distribution of trapped particle density on the absorbing hyperplane is finite. Notice, as expected from the equivalence with electrostatics, that this eventual hitting probability is also just the electric field of a point charge located at \( \vec{h}_0 \) in the presence of a grounded hyperplane at \( x_d = 0 \). We will return to this equivalence when we discuss first passage in the wedge geometry in Chap. 7.

### 3.3 Systematic Approach

As a counterpoint to the image method, we now obtain first-passage properties by the systematic Green’s function solution that was emphasized in the previous chapter.

#### 3.3.1 The Green’s Function Solution

We compute the Green’s function for the diffusion equation with the initial condition \( c(x, t = 0) = \delta(x - x_0) \) and boundary condition \( c(x = 0, t) = 0 \). After a Laplace transform, the diffusion equation becomes

\[
sc(x, s) - \delta(x - x_0) = Dc''(x, s).
\]

In each subdomain, \( x < x_0 \) and \( x > x_0 \), the solution is a linear combination of exponential functions. From the boundary condition at \( x = 0 \), the linear combination must be antisymmetric for \( x < x_0 \); for \( x > x_0 \) the boundary condition at \( x = \infty \) implies that only the decaying exponential occurs. Thus

\[
c_< (x, s) = A \sinh(\sqrt{s/D}x)
\]

\[
c_>(x, s) = B \exp(-\sqrt{s/D}x).
\]

Imposing continuity of the concentration at \( x = x_0 \) and also the joining condition \( D(c'_> - c'_<)|_{x=x_0} = -1 \), we obtain

\[
c(x, s) = \frac{1}{\sqrt{Ds}} \sinh \left( \sqrt{s/D} x_0 \right) e^{-\sqrt{s/D} x_0},
\]
with \( x_\leq = \max(x, x_0) \) and \( x_\geq = \min(x, x_0) \). Writing the sinh function in terms of exponentials, we can write this Green’s function in the more symmetric and physically revealing form

\[
c(x, s) = \frac{1}{\sqrt{4sD}} \left[ e^{+\sqrt{s/D}(x-x_0)} - e^{-\sqrt{s/D}(x+x_0)} \right],
\]

where the positive sign refers to \( c_\geq \) and the negative sign to \( c_\leq \). It is elementary to invert this Laplace transform and recover the image solution form of \( c(x, t) \) quoted in Eq. (3.2.1).

For biased diffusion, the Green’s function for the Laplace transformed convection-diffusion equation

\[
sc(x, s) - \delta(x-x_0) + vc(x, s)' = Dc(x, s)''
\]

has the general form \( c = Ae^{\alpha+x} + Be^{\alpha-x} \), with \( \alpha_{\pm} = (v \pm \sqrt{v^2 + 4Ds})/(2D) \). When the boundary conditions are imposed, the Green’s function reduces to

\[
c(x, s) = \begin{cases} 
A(e^{\alpha+x} - e^{\alpha-x})e^{\alpha-x_0}, & x < x_0; \\
A(e^{\alpha+x_0} - e^{\alpha-x_0})e^{\alpha-x}, & x > x_0.
\end{cases}
\]

Finally the constant \( A \) is obtained from the usual joining condition \( D(c'_\geq - c'_\leq)|_{x=x_0} = -1 \). Thus the Green’s function is

\[
c(x, s) = \begin{cases} 
\frac{1}{D(\alpha_+ - \alpha_-)}(e^{\alpha_+ x} - e^{\alpha_- x})e^{\alpha_+ x_0}, & x < x_0; \\
\frac{1}{D(\alpha_+ - \alpha_-)}(e^{\alpha_- x_0} - e^{-\alpha_+ x_0})e^{\alpha_- x}, & x > x_0.
\end{cases}
\]

From this, the flux to the origin is

\[
F(0, s) = +Dc'_\leq|_{x=0} = e^{-\alpha+x_0}.
\]

We now invert this Laplace transform to find the time dependence of the first-passage probability. For this, we use the general theorem that the inverse Laplace transform of the function \( f(s + a) \), equals \( e^{-at} \) times the inverse Laplace transform of \( f(s) \) (Ghez (1988)). That is, \( \mathcal{L}^{-1}(f(s + a)) = e^{-at} \mathcal{L}^{-1}(f(s)) \). For the present example,

\[
F(0, s) = e^{-vx_0/2D}e^{-(x_0/\sqrt{D})\sqrt{s+v^2/4D}},
\]

so that

\[
F(0, t) = e^{-vx_0/2D} \left[ e^{-v^2t/4D} \mathcal{L}^{-1}(e^{-x_0\sqrt{s/D}}) \right] = \frac{x_0}{\sqrt{4\pi Dt^3}} e^{-x_0^2/4Dt} e^{-vx_0/2D} e^{-v^2t/4D},
\]

which coincides with Eq. (3.2.13). Thus complete results for first-passage on the semi-interval can be obtained either by the Green’s function approach or by the intuitive image method.

### 3.3.2 Constant-Density Initial Condition

We now study the constant-density initial distribution because of its utility for diffusion-controlled reactions in a one-dimensional geometry, in which a chemical reactant is neutralized when it reaches \( x = 0 \). A simple example is particle-antiparticle annihilation \( A + B \rightarrow 0 \), where \( A \) initially occupies the region \( x > 0 \) and \( B \) occupies the region \( x < 0 \) (Galáfi & Rácz (1988)). Annihilation takes place within a thin reaction zone which is centered at \( x = 0 \). A first step in understanding this kinetics is provided by studying the simpler system where reactions occur exactly at \( x = 0 \).

The constant-density initial condition on \((0, \infty)\) can be solved either by the image method or by a direct solution of the diffusion equation; we present the latter approach. Thus we solve the diffusion equation subject to the initial condition \( c(x, t = 0) = c_0 \), and the boundary conditions \( c(x = 0, t) = 0 \) and \( c(x = \infty, t) = c_0 \).
The Laplace transform of the diffusion equation gives \( sc(x, s) - c_0 = Dc''(x, s) \), and, after the boundary conditions are applied, the solution is

\[
c(x, s) = \frac{c_0}{s}(1 - e^{-x\sqrt{s}}). \tag{3.3.6}
\]

Inverting the Laplace transform, the corresponding solution as a function of time is

\[
c(x, t) = c_0 \text{erf}\left(\frac{x}{\sqrt{4Dt}}\right). \tag{3.3.7}
\]

An important feature of this concentration profile is the gradual depletion of the density near the origin. This is reflected by the fact that the flux to the origin decreases with time as

\[
j(x = 0, t) = Dc'(x = 0, t) = \sqrt{\frac{D}{\pi t}} c_0. \tag{3.3.8}
\]

In the context of diffusion-controlled reactions, this means that the reaction rate at an absorbing boundary also decreases with time.

![Fig. 3.5. Concentration profile at \( Dt = 50, 250, 1250, \) and 6250 for an absorbing boundary at \( x = 0 \) and a constant initial concentration \( c_0 = 1 \) for \( x > 0 \).](image)

Notice that the concentration profile (see Fig. 3.5) for the uniform initial condition (Eq. (3.3.7)) is identical to the survival probability for the point initial condition (Eq. (3.2.9b)). This coincidence is no accident! It arises because the underlying calculations for these two results are, in fact, identical. Namely:

- For a particle initially at \( x_0 \), the survival probability \( S(t) \) is found by first calculating the concentration with this initial state, \( \delta(x - x_0) \), and then integrating the concentration over all \( x > 0 \) to find the survival probability.
- For an initial concentration equal to one for \( x > 0 \), we can view the initial condition of a superposition of delta functions. We then find the concentration for \( t > 0 \) by integrating the time-dependent concentration which arises at each such source over all space.
To show formally that these two computations are equivalent, define \( c(x, t; x_0) \) as the Green’s function for the diffusion equation on the positive semi-interval for a particle which is initially at \( x_0 \). Here we explicitly write the source point \( x_0 \) and the observation point \( x \). We now exploit the fact that this Green’s function satisfies the reciprocity relation

\[
c(x, t; x_0) = c(x_0, t; x)
\]

under the interchange of the source and the observation points. By definition, the survival probability for a particle which is initially at \( x_0 \) equals

\[
S(t; x_0) = \int_0^\infty c(x, t; x_0) \, dx.
\]

On the other hand, for the uniform initial condition, the time-dependent concentration is given by

\[
\int_0^\infty c(x, t; x_0) \, dx_0 = \int_0^\infty c(x_0, t; x) \, dx_0 \quad \text{(reciprocity)}
\]

\[
= \int_0^\infty c(x, t; x_0) \, dx \quad \text{(relabeling)}
\]

\[
= S(t; x_0),
\]

thus showing the equivalence of the concentration due to a uniform initial condition and the survival probability due to a point initial condition.

### 3.4 Discrete Random Walk

#### 3.4.1 The Reflection Principle

We now study first-passage properties of a symmetric nearest-neighbor random walk. Much of this discussion is based on the treatment given in Chap. III in Vol. I of Feller’s book (Feller (1968)). Although the results are equivalent to those of continuum diffusion, the methods of solution are appealing and provide the starting point for treating the intriguing origin crossing properties of random walks. We start by deriving the fundamental reflection principle which allows us to derive easily various first-passage properties in terms of the occupation probability.

It is convenient to view a random walk as a directed path in space-time \((x, t)\), with isotropic motion in space and directed motion in time (Fig. 3.6). Let \( N(x, t|x_0, 0) \) be the total number of random walks which start at \((x_0, 0)\) and end at \((x > x_0, t)\). Typically, we will not write the starting location dependence unless instructive. This dependence can always be eliminated by translational invariance, \( N(x, t|x_0, 0) = N(x - x_0, t|0, 0) \equiv N(x - x_0, t) \).

Consider a random walk which starts at \((0, 0)\), crosses a point \( y > x \), and then ends at \((x, t)\) (Fig. 3.6). Let \( X_y(x, t) \) be the number of these “crossing” paths between 0 and \( x \). The reflection principle states that

\[
X_y(x, t) = N(2y - x, t).
\]

This relation arises because any crossing path has a unique last visit to \( y \). We may then construct a “reflected” path by reversing the direction of all steps after this last visit (Fig. 3.6). It is clear that there is a one-to-one mapping between the crossing paths that comprise \( X_y(x, t) \) and these reflected paths. Moreover the reflected paths are unrestricted because \( y \) is necessarily crossed in going from \((0, 0)\) to \((2y - x, t)\). Thus the reflected paths constitute \( N(2y - x, t) \). Parenthetically, this reflection construction could also be applied to the leading segment of the crossing path to give the equality \( X_y(x, t) = N(x, t(2y, 0)) = N(2y - x, t) \).

#### 3.4.2 Consequences for First Passage

We now use this reflection principle to compute the number of first-passage paths \( F(x, t|0, 0) \), that is, paths which start at \((0, 0)\) and arrive at \((x, t)\) without previously touching or crossing \( x \). This is a pleasant,
Fig. 3.6. The reflection principle illustrated. The solid curve is a “crossing” path to \((x, t)\) by way of \((y, t')\), with \(t' < t\). The number of such restricted paths is the same as the number of unrestricted paths to \((2y - x, t)\). The reflected portion of the trajectory is shown as a dotted curve.

graphically-based computation (Fig. 3.7). First notice that \(F(x, t)\) is the same as \(F(x - 1, t - 1)\), as there is only one way to continue the first-passage path from \((x - 1, t - 1)\) to \((x, t)\). Next, the number of first-passage paths from \((0, 0)\) to \((x - 1, t - 1)\) can be written as the difference

\[
F(x - 1, t - 1) = N(x - 1, t - 1) - X_x(x - 1, t - 1),
\]

where again \(X_x(x - 1, t - 1)\) is the number of paths from \((0, 0)\) to \((x - 1, t - 1)\) which \textit{necessarily} touch or cross \(x\) before \(t - 1\) steps. By the reflection principle, \(X_x(x - 1, t - 1) = N(x + 1, t - 1)\). Consequently, the number of first-passage paths from \((0, 0)\) to \((x, t)\) after \(t\) steps is

\[
F(x, t) = F(x - 1, t - 1)
= N(x - 1, t - 1) - N(x + 1, t - 1)
= \frac{(t - 1)!}{\left(\frac{t + x - 2}{2}\right)! \left(\frac{t - x}{2}\right)!} \cdot \left(\frac{t + x - 2}{2}\right)! \left(\frac{t - x}{2}\right)! \cdot \frac{t!}{t! (t - 1)!}
= \frac{x}{t} N(x, t).
\]

Since the total number of paths from \((0, 0)\) to \((x, t)\) is proportional to \(e^{-x^2/4Dt}/\sqrt{4\pi Dt}\) in the continuum limit, the number of first-passage paths between these two points therefore scales as \(x e^{-x^2/4Dt^3}/\sqrt{4\pi Dt}\), in agreement with our previous derivations of this result.

If the endpoint is also at \(x = 0\), then we have the first return to the origin. In this case, we apply the reflection principle in a slightly different form to obtain the number of first-passage paths. Suppose that the first step is to the right. Then the last step must be to the left, and hence \(f(t) \equiv F(0, t) = F(1, t - 1|1, 1)\). The reflection principle now gives

\[
f(t) = F(1, t - 1|1, 1)
= N(1, t - 1|1, 1) - X_0(1, t - 1|1, 1)
= N(1, t - 1|1, 1) - N(1, t - 1 - 1, 1)
= \frac{(t - 2)!}{[(t/2 - 1)!]^2} \frac{(t - 2)!}{(t/2)! (t/2 - 2)!}.
\]
3.4 Discrete Random Walk

3.4.3 Origin Crossing Statistics

3.4.3.1 Qualitative Picture and Basic Questions

Hidden within the survival and the first-passage probabilities of the one-dimensional random walk are fundamental properties about the statistics of crossings of the origin (see Fig. 3.8). Some of these properties are sufficiently counter-intuitive that they appear to be “wrong”, yet they can be derived simply and directly.
from the first-passage probability. They dramatically illustrate the profound implications of the power-law tail in the first-passage probability of a random walk.

Consider a symmetric random walk on the infinite line. We have learned that the mean time for such a random walk to return to the origin is infinite (Eq. (3.2.5)); on the other hand, from Eq. (3.4.4), the probability of return to the origin after a relatively small number of steps is appreciable. For example, the first-passage probabilities \( f(t) \) are \( \frac{1}{2}, \frac{1}{8}, \frac{1}{16}, \frac{5}{128} \), and \( \frac{7}{256} \) for \( t = 2, 4, 6, 8, \) and \( 10 \), respectively. Thus the probability of returning to the starting point within 10 steps is 0.7539 \( \ldots \). This contrast between the relatively large probability of returning after a short time and an infinite mean return time is the source of the intriguing properties of origin crossings by a random walk.

We focus on two basic questions. First:

- What is the average number of returns to the origin in an \( n \)-step walk? More generally, what is the probability that there are \( m \) returns to the origin in an \( n \)-step walk?

Surprisingly, the outcome with the largest probability is zero returns. In fact, the probability for \( m \) returns in an \( n \)-step walk has the Gaussian form \( e^{-m^2/n} \), so that the typical number of returns after \( n \) steps is of the order of \( \sqrt{n} \) or less. Thus returns are relatively unlikely.

We also study the lead probability. To appreciate its meaning, consider again the coin-tossing game where player \( A \) wins $1 from \( B \) if a coin toss is heads and gives $1 to \( B \) if the result is tails. This is the same as a one-dimensional random walk, in which the position \( x \) of the walk at time \( t \) is the difference in the number of wins for \( A \) and \( B \). In a single game with \( n \) coin tosses, \( A \) will be leading for a time \( n \phi \), whereas \( B \) will be leading for a time \( n(1 - \phi) \). (In a discrete random walk, “ties” can occur; we can eliminate these by defining the leader in the previous step as the current leader.) This gives our second fundamental question:

- For an \( n \)-step random walk, what is the lead fraction \( \phi \)? What is the probability distribution for this lead fraction?

Amazingly, the lead fraction is likely to be close to 0 or 1! That is, one player is in the lead most of the time, even though the average amount won is zero! Conversely, the least likely outcome is the naive expectation that each player should be in the lead for approximately one-half the time.

The ultimate expression of these unexpected results is the beautiful arcsine law for the lead probability. To set the stage for this law, we first study the statistics of number of returns to the origin. We then treat the statistics of lead durations, from which the arcsine law follows simply.

### 3.4.3.2 Number of Returns to the Origin

It is easy to estimate the typical number of returns to the origin in an \( n \)-step walk. Since the occupation probability at the origin is \( P(n, 0) \propto 1/\sqrt{n} \), after \( n \) steps there are of the order of \( n/\sqrt{n} = \sqrt{n} \) returns. Accordingly, returns to the origin should be few and far between! In fact, returns to the origin are clustered
3.4 Discrete Random Walk

because the distribution of times between returns has a \( t^{-3/2} \) tail. Thus of the \( \sqrt{n} \) returns to the origin, most occur after a very short duration (Fig. 3.8).

Now let’s consider the probability that an \( n \)-step random walk contains \( m \) returns to the origin. This can be found conveniently in terms of the first- and the \( m \)-th passage probabilities of the random walk. Our treatment of multiple returns follows the discussion given in Weiss & Rubin (1983) and Weiss (1994). Let \( F(x, n) \) be the usual first-passage probability that a random walk, which starts at the origin, hits \( x \) for the first time at the \( n \)-th step. From Chap. 1, the generating function, \( F(x, z) = \sum_n F(x, n) z^n \), is

\[
F(x, z) = \frac{P(x, z) - \delta_{x,0}}{P(0, z)}, \quad (3.4.8)
\]

where \( P(x, z) \) is the generating function for the occupation probability \( P(x, n) \).

Now define the \( m \)-th-passage probability \( F^{(m)}(x, n) \) as the probability that a random walk hits \( x \) for the \( m \)-th time at the \( n \)-th step. This \( m \)-th-passage probability can be expressed recursively in terms of the \((m - 1)\)-th-passage probability

\[
F^{(m)}(x, n) = \sum_{k=0}^{n} F^{(m-1)}(x, k) F(0, n - k). \quad (3.4.9)
\]

That is, for the walk to hit \( x \) for the \( m \)-th time at step \( n \), it must hit \( x \) for the \((m - 1)\)-th time at an earlier step \( k \) and then return to \( x \) one more time exactly \( n - k \) steps later. This recursion is conceptually similar to the convolution which relates the first-passage probability to the occupation probability (Eq. (1.2.1)).

As usual, we can solve this recursion easily by substituting the generating function \( F^{(m)}(x, z) = \sum_n F^{(m)}(x, n) z^n \) into the above recursion formula to give \( F^{(m)}(x, z) = F^{(m-1)}(x, z) F(0, z) = F(x, z) F(0, z)^{m-1} \). Here we use the definition that \( F^{(1)}(x, z) = F(x, z) \). We therefore find

\[
F^{(m)}(x, z) = \begin{cases} 
\frac{P(x, z)}{P(0, z)} \left( \frac{P(x, z) - \delta_{x,0}}{P(0, z)} \right)^{m-1} & x \neq 0; \\
\left( 1 - \frac{1}{P(0, z)} \right)^m & x = 0.
\end{cases} \quad (3.4.10)
\]

What we seek, however, is the probability that \( x \) is visited \( m \) times sometime during an \( n \)-step walk. This \( m \)-visit probability can be obtained from the \( m \)-th-passage probabilities as follows. First, the probability that \( x \) has been visited at least \( m \) times in an \( n \)-step walk is

\[
\begin{align*}
&\sum_{j=1}^{n} F^{(m)}(x, j); \quad x \neq 0 \\
&\sum_{j=1}^{n} F^{(m-1)}(0, j). \quad x = 0
\end{align*} \quad (3.4.11)
\]

These express the fact that to visit \( x \) at least \( m \) times, the \( m \)-th visit must occur in \( j \leq n \) steps. Alternatively, we could sum \( F^{(m)}(x, n) \) from \( m \) to \( \infty \) to get the probability of visiting at least \( m \) times, but this formulation is less convenient for our purposes.

The probability that there are \( m \) visits to \( x \) sometime during an \( n \)-step walk, \( G^{(m)}(x, n) \), is just the difference in the probability of visiting at least \( m \) times and at least \( m + 1 \) times. Therefore

\[
G^{(m)}(x, n) = \begin{cases} 
\sum_{j=1}^{n} \left[ F^{(m)}(x, n) - F^{(m+1)}(x, n) \right] & x \neq 0 \\
\sum_{j=1}^{n} \left[ F^{(m-1)}(0, n) - F^{(m)}(0, n) \right] & x = 0.
\end{cases} \quad (3.4.12)
\]
In terms of the generating function for $G$, these relations become

$$G^{(m)}(x, z) = \begin{cases} 
\frac{1}{1-z} [F^{(m)}(x, z) - F^{(m+1)}(x, z)] & x \neq 0 \\
\frac{1}{1-z} [F^{(m-1)}(0, z) - F^{(m)}(0, z)] & x = 0.
\end{cases} \tag{3.4.13}$$

Let us now focus on returns to the origin. Substituting the $m$th-passage probability (Eq. (3.4.10)), and also the relation between the first-passage and occupation probabilities (Eq. (1.2.3)) into Eq. (3.4.13), we obtain

$$G^{(m)}(0, z) = \frac{1}{1-z} \left( 1 - \frac{1}{P(0, z)} \right)^m \frac{1}{P(0, z)} \tag{3.4.14}$$

It is easy to extract the asymptotic time dependence from this generating function. Using $P(0, z) = (1 - z^2)^{-1/2} \approx (2s)^{-1/2}$ as $z \to 1$ from below, with $s = 1 - z$, we have

$$G^{(m)}(0, s) \approx \frac{1}{s} (1 - \sqrt{2s})^m \sqrt{2s}$$

$$\sim \sqrt{\frac{2}{s}} e^{-m \sqrt{2s}}. \tag{3.4.15}$$

This is essentially identical to the Laplace transform of the random walk occupation probability in Eq. (1.3.22)!

Thus we conclude that the probability for a random walk to make $m$ visits to the origin during the course of an $n$-step walk is simply

$$G^{(m)}(0, n) \sim \frac{1}{\sqrt{2\pi n}} e^{-m^2/2n}. \tag{3.4.16}$$

We can obtain this same result more simply by noticing that Eq. (3.4.14), is essentially the same as the generating function for the occupation probability at displacement $x = m$ (Eq. (1.3.11)).

Eq. (3.4.16) has very amusing consequences. First, from among all the possible outcomes for the number of returns to the origin, the most likely outcome is zero returns. In the context of the coin-tossing game, this means that one person would always be in the lead. The probability for $m > 0$ returns to the origin monotonically decreases with $m$ and becomes vanishingly small after $m$ exceeds $\sqrt{n}$. Thus the typical number of returns is of the order of $\sqrt{n}$. As a result, ties in the coin-tossing game occur with progressively lower frequency as the game continues, since it is very unlikely that the number of returns is of the order of $n$.

### 3.4.3.3 Lead Probability and the Arcsine Law

We now turn to the lead probability of a random walk. The basic phenomenon is illustrated in Fig. 3.9. For a random walk of $n$ steps, a total of $k$ steps lie in the region $x > 0$, while the other $n - k$ steps lie in the region $x < 0$. If $x$ happens to be zero, we again use the tie-breaker rule of Subsection 3.4.3.1 – a walk at the origin is considered as having $x \gtrless 0$ if the location at the previous step was positive (negative). We want to find the probability $Q_{n,k}$ for this division of the lead times in an $n$-step walk.

We use the fact that the occurrence probabilities for each of the first-passage segments of the walk in Fig. 3.9 are independent. Hence they can be interchanged freely without changing the overall occurrence probability of the walk. We therefore move all the negative segments to the beginning and all the positive segments to the end. This rearranged walk can be viewed as composite of a return segment of length $n - k$ and a no-return segment of length $k$. For convenience, we now choose $n$ to be even while $k$ must be even. The occurrence probability of this composite path is just the product of the probabilities for the two constituents. From Eq. (3.4.5), the probability of the return segment is $R(k)/2^k$, while that of the no-return segment is $R(n-k)/2^{n-k}$. Thus the probability for all paths which are decomposable as in Fig. 3.9 is

$$Q_{n,k} = 2^{-n} R(k) R(n-k)$$

$$\sim \frac{1}{\pi \sqrt{k(n-k)}}. \tag{3.4.17}$$
As advertised previously, this probability is maximal for $k \to 0$ or $k \to n$ and the minimum value of the probability occurs when $k = n/2$. For large $n$,

$$Q_{n,k} \to Q(x) = \frac{1}{n\pi} \frac{1}{\sqrt{x(1-x)}}, \quad (3.4.18)$$

where $Q(x)$ is the probability that the lead fraction equals $x$ in an $n$-step walk.

In addition to the probability that player $A$ is in the lead for exactly $k$ out of $n$ steps, consider the probability $L_{k,n}$ that $A$ is in the lead for at least $k$ steps. In the limit $k, n \to \infty$ with $x = k/n$ remaining finite, $L_{n,k} \to L(x)$ becomes

$$L(x) = \int_{0}^{k} \frac{dk'}{\pi \sqrt{k'(n-k')}} = \frac{2}{\pi} \sin^{-1}\sqrt{x}, \quad (3.4.19)$$

where $x = k/n$. This is the continuous arcsine distribution.

The strange consequences of this arcsine distribution arise from the fact that the underlying density $1/\sqrt{x(1-x)}$ has a square-root singularity near the extremes of $x \to 0$ and $x \to 1$, as shown in Fig. 3.10. It is easy to devise paradoxical numerical illustrations of this distribution and many are given in Feller’s book (Feller (1968)). One nice example is our two-person coin tossing game which is played once every second for 1 year. Then, with probability 1/2, the unluckier player, which could be either $A$ or $B$, will be leading in this game for 53.45 days or fewer – that is, less than 0.146 of the total time. With probability 1/10 (inset of Fig. 3.10), the unluckier player will be leading for 2.24 days or fewer – less than 0.00615 of the total time!

As a final note, when there is a finite bias in the random walk, almost all of the subtleties associated with the tension between certain return and infinite return time disappear. A random walk becomes aware of its
Fig. 3.10. The arcsine distribution. Shown are both the underlying density $nQ(x)$ (upper curve), and the arcsine distribution itself $L(x)$ (lower curve). The inset shows $L(x)$ near $x = 0$. The dashed line highlights the numerical example that, at $x \approx 0.00615$, $L(x)$ has already risen to 0.05.

bias once the Péclet number becomes large. Beyond this point, all the dynamics is controlled by the bias and a gambler on the wrong side of the odds will always be losing.

### 3.5 Imperfect Absorption

#### 3.5.1 Motivation

We now investigate the role of imperfect boundary absorption on first-passage and related properties of diffusion on the semi-infinite interval. Imperfect absorption means that a random walk may be either reflected or absorbed when it hits the origin. In the continuum limit, this leads naturally to the radiation boundary condition, in which the concentration is proportional to the flux at $x = 0$. This interpolates between the limiting cases of perfect absorption and perfect reflection as the microscopic absorption rate is varied. We will discuss basic physical features of this radiation boundary condition and also discuss how imperfect absorption in the semi-infinite interval is equivalent to perfect absorption in the long-time limit.

From a physical perspective, we will also show that a semi-infinite system with a radiation boundary condition is equivalent to an infinite system with free diffusion for $x > 0$ and attenuation for $x < 0$ (Ben-Naim et al. (1993b)). The latter provides a simple model for the propagation of light in a turbid medium, such as a concentrated suspension or human tissue. A general discussion of this phenomenon is given in Chap. 7 of Weiss (1994). This equivalence means that we can understand properties of diffusive propagation inside an attenuating medium in terms of the concentration outside the medium.
3.5.2 Radiation Boundary Condition

To see how the radiation boundary condition arises, consider a discrete random walk on \( x \geq 0 \) with a probability \( p \) of hopping to the right and \( q \) to the left (see Fig. 3.11). Let \( P(i, n) \) be the probability that the particle is at site \( i \) at the \( n^{th} \) time step. For \( i \geq 2 \), the occupation probabilities obey the master equations

\[
P(i, n + 1) = pP(i - 1, n) + qP(i + 1, n),
\]

while the master equation for site \( i = 1 \) is distinct because the boundary site \( i = 0 \) alters the rate at which probability from site 0 reaches 1.

![Diagram of absorbing, reflecting, and radiation boundary conditions](image)

Fig. 3.11. Illustration of (a) absorbing, (b) reflecting, and (c) radiation boundary conditions. The solid arrows denote the bulk hopping probabilities, and the dashed arrow denotes the hopping probability from the origin to site 1.

To set the stage for the radiation condition, consider first the absorbing and reflecting boundary conditions. For an absorbing boundary, a particle is absorbed once it reaches site 0 and there is no flux from site 0 to 1. Consequently, the master equation for site 1 is simply

\[
P(1, n + 1) = qP(2, n).
\]

This idiosyncratic equation can be recast in the same form as Eqs. (3.5.1) if the absorbing boundary condition \( P(0, n) = 0 \) is imposed. In the continuum limit, this clearly translates to zero interface concentration, \( c(0, t) = 0 \).

For the reflecting boundary, the net probability flux across bond \((i, i+1)\) at the \( n^{th} \) step is simply

\[
j_{i,i+1} = pP(i, n) - qP(i + 1, n).
\]

Zero flux at the boundary means that \( pP(0, n) = qP(1, n) \). We can write the flux in a more useful form by defining \( p = \frac{1}{2} + \epsilon \) and \( q = \frac{1}{2} - \epsilon \), so that

\[
j_{i,i+1}(n) = (\frac{1}{2} + \epsilon)P(i, n) - (\frac{1}{2} - \epsilon)P(i + 1, n)
\]

\[
= \frac{1}{2} (P(i, n) - P(i + 1, n)) + \epsilon (P(i, n) + P(i + 1, n)).
\]

By Taylor expanding, we obtain the familiar continuum expression for the flux \( j(x, t) = -D \frac{\partial c(x, t)}{\partial x} + vc(x, t) \), with diffusion coefficient \( D = 1/2 \) and velocity \( v = 2\epsilon \). For an isotropic random walk, the reflecting boundary condition therefore leads to a zero concentration gradient at the interface.
Finally, we turn to the boundary condition for partial absorption and partial reflection. There is subtlety in formulating the simplest situation that quickly leads to the correct result, as discussed thoroughly in Weiss (1994). We adopt the simple choice that if the random walk hops to the left from site 1, it is reflected and immediately returned to site 1 with probability $r$, while with probability $1 - r$ the walk is trapped permanently at site 0. This means that the net flux to site 0 is simply $j_{0,1}(n) = -(1 - r)qP(1, n)$ (Fig. 3.11(c)). On the other hand, comparing this with the general form of the flux in Eq. (3.5.3) leads to $pP(0, n) = rqP(1, n)$. By Taylor expanding this relation to lowest order, we find the radiation boundary condition for isotropic diffusion,

$$\frac{\partial c(x, t)}{\partial x} \bigg|_{x=0} = \kappa c(0, t),$$

(3.5.5)

where $\kappa = (1 - r)/r\Delta x$ has the units of an inverse length.

To appreciate the physical meaning of the radiation boundary condition, consider diffusion in the one-dimensional domain $x > 0$, subject to the radiation boundary condition at $x = 0$ and the initial condition $c(x, t = 0) = c_0$ for $x > 0$. This problem is easily solved in the Laplace domain, and the resulting time-dependent concentration is

$$c(x, t) = c_0 \text{erf} \left( \frac{x}{\sqrt{4Dt}} \right) + c_0 e^{(\kappa x + \kappa^2 Dt)} \text{erfc} \left( \frac{x}{\sqrt{4Dt}} + \kappa \sqrt{Dt} \right).$$

(3.5.6)

Fig. 3.12. Concentration $c(x, t)$ in Eq. (3.5.6) vs. $x$ for $Dt = 10, 100, 1000, \text{ and } 10000$ (top to bottom), with $\kappa = 0.1$ and $c_0 = 1$. In the range $x < 20$, the linear extrapolations of these curves to the $x$ axis approaches $-10$ as $t$ increases (arrow). The dashed line shows this extrapolation for the case $Dt = 1000$.

In the long-time limit, this solution smoothly approaches that of an absorbing boundary, as illustrated in Fig. 3.12. There are, however, two vestiges of the radiation boundary condition as $t \to \infty$. First, at $x = 0$ the concentration is not zero, but rather approaches zero as $c_0/\kappa \sqrt{Dt}$. Second, the concentration linearly extrapolates to zero at $x = -1/\kappa$. For $\kappa \gg 1$, the interface concentration and the extrapolation length $\ell \equiv 1/\kappa$ are both small and the boundary condition is close to perfectly absorbing. Conversely, for $\kappa \ll 1$, the concentration remains nearly constant and the boundary condition is nearly reflecting.
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The finite extrapolation length is suggestive of a “hidden” non-zero concentration in the region $x < 0$. We now discuss how to turn this vague observation into a mapping between the semi-infinite system with a radiating boundary, and an infinite composite medium with free diffusion for $x > 0$ and attenuation for $x < 0$.

3.5.3 Connection to a Composite Medium

A practical example of a composite medium with attenuation for $x < 0$ and free diffusion for $x > 0$ is the propagation of light in human tissue. In various diagnostic situations, laser light is incident upon a sample and some fraction of this incident light eventually re-emerges. Diffusion with attenuation provides a simple description for propagation in the sample, and useful information about its physical properties may be gained from the intensity and spatial distribution of the re-emitted light. Various practical aspects of this system are reviewed in Weiss (1994), see also Ishimaru (1978); Bonner et al. (1987) for additional details. While the real system is three dimensional, we discuss a one-dimensional composite because it illustrates the main features of diffusion with attenuation and it is easily soluble (Ben-Naim et al. (1993b)).

Fig. 3.13. Illustration of the correspondence between (a) a semi-infinite system $x > 0$ with a radiation boundary condition at $x = 0$, and (b) an infinite system with free propagation for $x > 0$ and attenuation for $x < 0$.

3.5.3.1 Diffusion-Absorption Equation

For diffusion in an unbounded one-dimensional medium, with attenuation at rate $q$ for $x < 0$ and free propagation for $x > 0$, the concentration is described by a diffusion-absorption equation for $x < 0$, and the diffusion equation for $x > 0$ (see Fig. 3.13),

\[
\begin{align*}
\frac{\partial c(x,t)}{\partial t} &= D \frac{\partial^2 c(x,t)}{\partial x^2} - qc(x,t), & x < 0, \\
\frac{\partial c(x,t)}{\partial t} &= D \frac{\partial^2 c(x,t)}{\partial x^2}, & x > 0.
\end{align*}
\]  
(3.5.7)
3.5.3.1.1 Single Particle Initial Condition It is simplest to locate the particle initially at the origin because it renders the Laplace transforms of Eqs. (3.5.7) homogeneous. The general solutions to these equations in each subdomain are then the single exponentials $c_+(x,s) = Ae^{-x\sqrt{s/D}}$, for $x > 0$, and $c_-(x,s) = Be^{x\sqrt{(s+q)/D}}$, for $x < 0$. By applying the joining conditions of continuity of the concentration and $D(c'_+ - c'_-)|_{x=0} = -1$, we obtain

$$
c(x,s) = \begin{cases} 
\frac{1}{\sqrt{Ds}} \frac{1}{1 + \alpha(s)} \exp \left( x\sqrt{(s+q)/D} \right) & x < 0, \\
\frac{1}{\sqrt{Ds}} \frac{1}{1 + \alpha(s)} \exp \left( - x\sqrt{s/D} \right) & x > 0,
\end{cases}
$$

(3.5.8)

where $\alpha(s) = \sqrt{(s + q)/s}$.

To appreciate the meaning of these results, let us focus on the following characteristic quantities of penetration into the attenuating medium:

- The survival probability, $S(t) = \int_{-\infty}^{+\infty} c(x,t) dx$.
- The total concentration within the absorbing medium, defined as $C_-(t) = \int_{-\infty}^{0} c(x,t) dx$.
- The concentration at the origin.

The first two quantities are simply related. By integrating the first of Eqs. (3.5.7) over the half space $x < 0$, we find

$$
\frac{dC_-(t)}{dt} = D \frac{\partial c(x,t)}{\partial x} \bigg|_{x=0} - qC_-(t).
$$

(3.5.9)

Thus $C_-(t)$ decreases because of absorption within $x < 0$, but is replenished by flux entering at $x = 0$. Additionally, by adding to Eq. (3.5.9) the result of integrating the second of Eqs. (3.5.7) over all $x > 0$, we find $\dot{S}(t) = -qC_-(t)$.

From the concentration in Eq. (3.5.8), we obtain the basic observables in the time domain

$$
S(t) = I_0(t/2t_q) e^{-t/2t_q},
$$

$$
C_-(t) = \frac{1}{2} \left[ I_0(t/2t_q) - I_1(t/2t_q) \right] e^{-t/2t_q},
$$

$$
c(x = 0, t) = \frac{t_q}{\sqrt{4\pi Dt_q^3}} \left( 1 - \exp(-t/t_q) \right),
$$

(3.5.10)

where $I_n(x)$ is the modified Bessel function of the first kind of order $n$ (Abramowitz & Stegun (1972)), and $t_q = 1/q$ is the characteristic absorption time of the medium. For short times $t \ll t_q$, the survival probability is close to one, while the total probability in the attenuating medium grows linearly with time because of the initial diffusive penetration. Correspondingly, the density at the origin decreases as $(4\pi Dt)^{-1/2}$, as in pure diffusion. In this short-time limit, attenuation does not yet play a role.

Conversely, from the large-$z$ expansion

$$
I_n(z) = \frac{e^z}{\sqrt{2\pi}z} \left( 1 - \frac{n-1}{8z} + \ldots \right)
$$

we obtain the long-time behaviors for $t/t_q \to \infty$,

$$
S(t) \sim (t_q/\pi t)^{1/2},
$$

$$
C_-(t) \sim \frac{1}{2\sqrt{\pi}} (t_q/t)^{3/2}.
$$

(3.5.11)

Here the survival probability decays as if there were a perfect absorber at the origin. This arises because a diffusing particle makes arbitrarily long excursions into the attenuating medium so that the attenuation
3.6 The Quasi-Static Approximation

will eventually be total. It is in this sense that an attenuating medium has the same effect as a perfectly absorbing medium in the long-time limit.

3.5.3.1.2 Uniform Initial Condition For the initial condition, \( c(x, t = 0) = c_0 \) for \( x > 0 \) and \( c(x, t = 0) = 0 \) for \( x < 0 \), the Laplace transform of the concentration is

\[
\begin{align*}
    c(x, s) &= \begin{cases} 
    c_0 \frac{1}{s} \exp(x\sqrt{(s+q)/D}) & x < 0, \\
    c_0 \left(1 - \frac{1}{1 + \alpha(s)^{-1}}\exp(-x\sqrt{s/D})\right) & x > 0, 
    \end{cases}
\end{align*}
\]

from which we find the time dependences

\[
\begin{align*}
    c(0, t) &= \frac{c_0}{2} \left[ I_0(t/2t_q) + I_1(t/2t_q) \right] e^{-t/2t_q} \rightarrow \frac{c_0}{\sqrt{\pi t/t_q}} \quad t \gg t_q \\
    C_{-}(t) &= \frac{c_0 \ell}{\sqrt{\pi t/t_q}} \left(1 - e^{-t/t_q}\right) \rightarrow \frac{c_0 \ell}{\sqrt{\pi t/t_q}} \quad t \gg t_q.
\end{align*}
\]

Here \( \ell = \sqrt{D/q} = \sqrt{Dt_q} \) is the typical distance that a particle travels in the attenuating medium before being absorbed. We will show that this distance coincides with the previously-introduced extrapolation length. Notice also that the concentration at the origin is proportional to the total concentration inside the absorber, \( c(x = 0, t) \sim C_{-}(t)/\ell \).

Finally, by using Eq. (3.5.9) and neglecting the subdominant time derivative term in this equation, we find that the flux to the origin is, asymptotically

\[
D \frac{\partial c(x, t)}{\partial x} \bigg|_{x=0} \sim qC_{-}(t) \sim Dc_0/\sqrt{\pi Dt},
\]

Thus in the long-time limit, the flux to the origin is the same as that to a perfect trap. This is another example of how the region \( x < 0 \) becomes infinitely attenuating as \( t \to \infty \).

3.5.4 Equivalence to the Radiation Boundary Condition

We now deduce the basic equivalence between an infinite composite medium and a semi-infinite medium with a radiation boundary condition at \( x = 0 \). From the previous results for \( c(0, t) \) and the gradient at the origin, the concentration near the interface has the asymptotic behavior

\[
c(x, t) \sim \frac{c_0}{\sqrt{\pi t/t_q}} + \frac{c_0}{\sqrt{\pi q D t}} x, \quad t \gg t_q.
\]

This has the same qualitative form as the concentration for diffusion near a radiating boundary (see Fig. 3.12). In fact, from approximation (3.5.15) the interface concentration and its derivative are simply related by

\[
D \frac{\partial c(x, t)}{\partial x} \bigg|_{x=0} = \sqrt{Dq} c(0, t).
\]

This is just the radiation boundary condition! By comparing with Eq. (3.5.5), we also infer that \( \kappa = \sqrt{q/D} = 1/\ell \), so that the attenuation and the extrapolation lengths are the same.

3.6 The Quasi-Static Approximation

3.6.1 Motivation

We close our discussion of first passage in a semi-infinite domain by presenting the quasi-static approximation (see e.g., Reiss et al. (1977)). This simple approach provides an appealing and versatile way to bypass many technical complications in determining the concentration profile in complex boundary-value problems (see Fig. 3.14). The physical basis of this approximation is that the system can be divided into a “far” region, where the concentration has not yet been influenced by the boundary, and a complementary “near”
region, where diffusing particles can explore this zone thoroughly. In this near zone, the concentration should therefore be almost steady, or quasi-static, and can be described accurately by the time-independent (and simpler) Laplace equation, rather than by the diffusion equation. Then by matching the near and far solutions, we obtain the global solution. This approach is now described for both the absorbing and radiation boundary conditions.

\[ c(\mathbf{r}, t) \]

Fig. 3.14. Schematic illustration of the quasi-static approximation for an absorbing boundary condition. The respective near-zone (solid curve) and far-zone (dashed curve) concentrations match at \( r = r^* \approx \sqrt{Dt} \).

**3.6.2 Quasi-Static Solution at an Absorbing Boundary**

We consider the trivial (and previously-solved) concentration profile in the one-dimensional domain \( x > 0 \) for the initial condition \( c(x, t=0) = 1 \) for \( x > 0 \) and with absorption at \( x = 0 \). Although the exact solution is nearly as easy to obtain as the quasi-static solution, the latter is much more versatile and can be easily applied to the same geometry in higher dimensions, while the exact solution is much more difficult to obtain. A specific illustration of this is given in Subsection 6.5.4.

According to the quasi-static approximation, we first identify the spatial domain \( 0 < x < \sqrt{Dt} \) as the near zone, where the concentration obeys the Laplace equation \( c'' = 0 \). Conversely, in the far zone \( x > \sqrt{Dt} \), the concentration remains at its initial value. The subtle issue is how to match the solutions from these two zones. The simplest approach is to adjust the amplitude of the near-zone solution so that it equals the far zone solution at \( x^* = \sqrt{Dt} \). Since \( x^* \) has a time dependence, this matching induces a time dependence into the Laplacian solution. Thus the near zone concentration profile is actually quasi-static, since it is the solution to the Laplace equation with a time-dependent boundary condition. However, this moving boundary condition is generally easy to apply because of the simplicity of the near-zone solution.

For our example, the near zone solution is simply \( c(x, t)_{\text{near}} = A + Bx \), and we determine \( A \) and \( B \) by imposing the absorbing boundary condition \( c(0, t) = 0 \) and the matching condition \( c(x = \sqrt{Dt}, t) = 1 \). These immediately give

\[
  c(x, t) \simeq \begin{cases} 
  \frac{x}{\sqrt{Dt}} & \text{for } 0 < x < \sqrt{Dt} \\
  1 & \text{for } x > \sqrt{Dt}.
\end{cases}
\]  

(3.6.1)

This simple form reproduces the basic features of the exact solution given in Eq. (3.3.7). In particular, the flux to the origin decays as \( \sqrt{D/t} \), compared to the exact result of \( \sqrt{D/\pi t} \).

**3.6.3 Quasi-Static Solution at a Radiation Boundary**

For a radiation boundary condition in one dimension, we again solve the Laplace equation in the near zone \( 0 < x < \sqrt{Dt} \), and match it to the constant far zone concentration at \( x = \sqrt{Dt} \). The near-zone solution is
now subject to the radiation boundary condition $Dc' = \sqrt{Dqc}|_{x=0}$ (Eq. (3.5.16)). By applying this boundary condition and the matching condition at $x = \sqrt{Dt}$ to the generic near-zone solution, $c(x, t)_{\text{near}} = A + Bx$, we easily find

$$c(x, t)_{\text{near}} = \frac{c_0}{1 + \sqrt{t/t_q}} \left(1 + \frac{x}{\ell}\right).$$

(3.6.2)

It is easy to verify that this very simple result reproduces the main features of the exact concentration profile near a radiating boundary. Namely, the concentration at the interface asymptotically decays as $\sqrt{t_q/t}$, the slope of the concentration at the interface is $1/\sqrt{Dt}$, and the concentration profile extrapolates to zero at $x = -\ell$. 