This is very similar to the solution of the time-independent Ornstein-Uhlenbeck process, as derived in Sect. 4.5.6, equation (4.5.53).

From this we have

$$\langle \boldsymbol{x}(t) \rangle = \exp\Big[-\int_0^t A(t')\,dt' \Big] \langle \boldsymbol{x}(0) \rangle , \tag{4.5.110}$$

$$\langle \boldsymbol{x}(t), \boldsymbol{x}^{\mathrm{T}}(t) \rangle = \exp\Big[-\int_0^t A(t')\,dt' \Big] \langle \boldsymbol{x}(0), \boldsymbol{x}(0)^{\mathrm{T}} \rangle \exp\Big[-\int_0^t A^{\mathrm{T}}(t')\,dt' \Big] + \int_0^t dt' \exp\Big[-\int_{t'}^t A(s)ds \Big] B(t') B^{\mathrm{T}}(t') \exp\Big[-\int_t^t A^{\mathrm{T}}(s)ds \Big]. \tag{4.5.111}$$

The time-dependent Ornstein-Uhlenbeck process will arise very naturally in connection with the development of asymptotic methods in low-noise systems.

5. The Fokker-Planck Equation

In the next two chapters, the theory of continuous Markov processes is developed from the point of view of the corresponding Fokker-Planck equation, which gives the time evolution of the probability density function for the system. This chapter is devoted mainly to single variable systems, since there are a large number of exact results for single variable systems, which makes the separate treatment of such systems appropriate. The next chapter deals with the more general multivariable aspects of many of the same issues treated one-dimensionally in this chapter.

The construction of appropriate boundary conditions is of fundamental importance, and is carried out in Sect. 5.1 in a form applicable to both one-variable and many-variable systems. A corresponding treatment for the boundary conditions on the backward Fokker-Planck equation is given in Sect. 5.1.2. The remaining of the chapter is devoted to a range of exact results, on stationary distribution functions, properties of eigenfunctions, and exit problems, most of which can be explicitly solved in the one variable case.

We have already met the Fokker-Planck equation in several contexts, starting from Einstein's original derivation and use of the diffusion equation (Sect. 1.2), again as a particular case of the differential Chapman-Kolmogorov equation (Sect. 3.5.2), and finally, in connection with stochastic differential equations (Sect. 4.3.5). There are many techniques associated with the use of Fokker-Planck equations which lead to results more directly than by direct use of the corresponding stochastic differential equation; the reverse is also true. To obtain a full picture of the nature of diffusion processes, one must study both points of view.

The origin of the name "Fokker-Planck Equation" is from the work of *Fokker* (1914) [5.1, 5.2] and *Planck* (1917) [5.2] where the former investigated Brownian motion in a radiation field and the latter attempted to build a complete theory of fluctuations based on it. Mathematically oriented works tend to use the term "Kolmogorov's Equation" because of Kolmogorov's work in developing its rigorous basis [5.3]. Yet others use the term "Smoluchowski Equation" because of Smoluchowski's original use of this equation. Without in any way assessing the merits of this terminology, I shall use the term "Fokker-Planck equation" as that most commonly used by the audience to whom this book is addressed.

5.1 Probability Current and Boundary Conditions

The FPE is a second-order parabolic partial differential equation, and for solutions we need an initial condition such as (5.2.5) and boundary conditions at the end of the interval inside which x is constrained. These take on a variety of forms.

It is simpler to derive the boundary conditions in general, than to restrict consideration to the one variable situation. We consider the forward equation

$$\partial_t p(z,t) = -\sum_i \frac{\partial}{\partial z_i} A_i(z,t)p(z,t) + \tfrac{1}{2}\sum_{i,j}\frac{\partial^2}{\partial z_i \partial z_i} B_{ij}(z,t)p(z,t)\,. \tag{5.1.1}$$

We note that this can also be written

$$\frac{\partial p(z,t)}{\partial t} + \sum_i \frac{\partial}{\partial z_i} J_i(z,t) = 0\,, \tag{5.1.2}$$

where we define the *probability current*

$$J_i(z,t) = A_i(z,t)p(z,t) - \tfrac{1}{2}\sum_j \frac{\partial}{\partial z_j} B_{ij}(z,t)p(z,t)\,. \tag{5.1.3}$$

Equation (5.5) has the form of a local conservation equation, and can be written in an integral form as follows. Consider some region R with a boundary S and define

$$P(R,t) = \int_R dz\, p(z,t)\,, \tag{5.1.4}$$

then (5.1.2) is equivalent to

$$\frac{\partial P(R,t)}{\partial t} = -\int_S dS\; \boldsymbol{n}\cdot \boldsymbol{J}(z,t)\,, \tag{5.1.5}$$

where $\boldsymbol{n}$ is the outward pointing normal to S. Thus (5.1.5) indicates that the total loss of probability is given by the surface integral of $\boldsymbol{J}$ over the boundary of R.

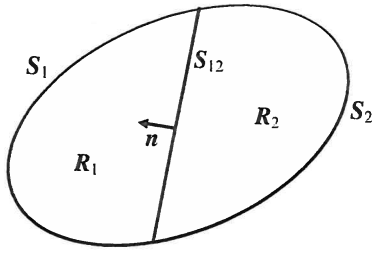

Fig. 5.1. Regions used to demonstrate that the probability current is the flow of probability

We can show as well that the current $\boldsymbol{J}$ does have the somewhat stronger property, that a surface integral over any surface S gives the net flow of probability across that surface. For consider two adjacent regions R_1 and R_2, separated by a surface S_{12}. Let S_1 and S_2 be the surfaces which, together with S_{12}, enclose respectively R_1, and R_2 (see Fig. 5.1).

Then the net flow of probability can be computed by noting that we are dealing here with a process with continuous sample paths, so that, in a sufficiently short time Δt, the probability of crossing S_{12} from R_2 to R_1 is the joint probability of being in R_2 at time t and R_1, at time $t+\Delta t$,

$$= \int_{R_1} d\boldsymbol{x} \int_{R_2} d\boldsymbol{y}\, p(\boldsymbol{x}, t+\Delta t; \boldsymbol{y}, t)\,. \tag{5.1.6}$$

The *net flow* of probability from R_2 to R_1 is obtained by subtracting from this the probability of crossing in the reverse direction, and dividing by Δt; i.e.

$$\lim_{\Delta t\to 0}\frac{1}{\Delta t}\int_{R_1} d\boldsymbol{x}\int_{R_2} d\boldsymbol{y}\,[p(\boldsymbol{x},t+\Delta t;\boldsymbol{y},t) - p(\boldsymbol{y},t+\Delta t;\boldsymbol{x},t)]\,. \tag{5.1.7}$$

Note that

$$\int_{R_1} d\boldsymbol{x}\int_{R_2} d\boldsymbol{y}\, p(\boldsymbol{x},t;\boldsymbol{y},t) = 0 \tag{5.1.8}$$

since this is the probability of being in R_1 and R_2 simultaneously. Thus, we can write

$$(5.1.7) = \int_{R_1} d\boldsymbol{x}\int_{R_2} d\boldsymbol{y}\,[\partial_{t'} p(\boldsymbol{x},t';\boldsymbol{y},t) - \partial_{t'} p(\boldsymbol{y},t';\boldsymbol{x},t)]_{t'=t}\,, \tag{5.1.9}$$

and using the Fokker-Planck equation in the form (5.5)

$$= -\int_{R_1} d\boldsymbol{x}\sum_i \frac{\partial}{\partial x_i} J_i(\boldsymbol{x},t;R_2,t) + \int_{R_2} d\boldsymbol{y}\sum_i \frac{\partial}{\partial y_i} J_i(\boldsymbol{y},t;R_1,t)\,, \tag{5.1.10}$$

where $J_i(\boldsymbol{x},t;R_2,t)$ is formed from

$$p(\boldsymbol{x},t;R_2,t) = \int_{R_2} d\boldsymbol{y}\, p(\boldsymbol{x},t;\boldsymbol{y},t)\,, \tag{5.1.11}$$

in the same way as $\boldsymbol{J}(z,t)$ is formed from $p(z,t)$ in (5.1.3) and $J_i(\boldsymbol{y},t;R_1 t)$ is defined similarly. We now convert the integrals to surface integrals. The integral over S_2 vanishes, since it will involve $p(\boldsymbol{x},t;R_2,t)$, with $\boldsymbol{x}$ not in R_2 or on its boundary (except for a set of measure zero.) Similarly the integral over S_1 vanishes, but those over S_{12} do not, since here the integration is simply over part of the boundaries of R_1 and R_2.

Thus we find, the net flow from R_2 to R_1 is

$$\int_{S_{12}} dS\; \boldsymbol{n}\cdot\{\boldsymbol{J}(\boldsymbol{x},t;R_1,t) + \boldsymbol{J}(\boldsymbol{x},t;R_2,t)\}\,, \tag{5.1.12}$$

and we finally conclude, since $\boldsymbol{x}$ belongs the union of R_1 and R_2, that the net flow of probability per unit time from R_2 to R_1

$$\equiv \lim_{\Delta t\to 0}\frac{1}{\Delta t}\int_{R_1} d\boldsymbol{x}\int_{R_2} d\boldsymbol{y}\Big[p(\boldsymbol{x},t+\Delta t;\boldsymbol{y},t) - p(\boldsymbol{y},t+\Delta t;\boldsymbol{x},t)\Big] = \int_{S_{12}} dS\,\boldsymbol{n}\cdot\boldsymbol{J}(\boldsymbol{x},t)\,,$$
where $\boldsymbol{n}$ points from R_2 to R_1. (5.1.13)

5.1.1 Classification of Boundary Conditions

We can now consider the various kinds of boundary condition separately.

a) Reflecting Barrier: We can consider the situation where the particle cannot leave a region R, hence there is zero net flow of probability across S, the boundary of R. Thus we require

$$\boldsymbol{n}\cdot\boldsymbol{J}(z,t)=0\,,\quad \text{for } z\in\boldsymbol{S},\quad \boldsymbol{n}=\text{normal to }\boldsymbol{S}\,, \tag{5.1.14}$$

where $\boldsymbol{J}(z,t)$ is given by (5.5.4).

Since the particle cannot cross $\boldsymbol{S}$, it must be reflected there, and hence the name *reflecting barrier* for this condition.

b) Absorbing Barrier: Here, one assumes that the moment the particle reaches $\boldsymbol{S}$, it is removed from the system, thus the barrier absorbs. Consequently, the probability of being on the boundary is zero, i.e.

$$p(z,t)=0\,,\qquad \text{for } z\in\boldsymbol{S}\,. \tag{5.1.15}$$

c) Boundary Conditions at a Discontinuity: It is possible for both the A_i and B_{ij} coefficients to be discontinuous at a surface $\boldsymbol{S}$, but for there to be free motion across $\boldsymbol{S}$. Consequently, the probability and the normal component of the current must both be continuous across $\boldsymbol{S}$,

$$\boldsymbol{n}\cdot\boldsymbol{J}(z)|_{S_+}=\boldsymbol{n}\cdot\boldsymbol{J}(z)|_{S_-}\,, \tag{5.1.16}$$

$$p(z)|_{S_+}=p(z)|_{S_-}\,, \tag{5.1.17}$$

where $\boldsymbol{S}_+,\boldsymbol{S}_-$, as subscripts, mean the limits of the quantities from the left and right hand sides of the surface.

The definition (5.1.3) of the current, indicates that the derivatives of $p(z)$ are not necessarily continuous at $\boldsymbol{S}$.

5.1.2 Boundary Conditions for the Backward Fokker-Planck Equation

We suppose that $p(\boldsymbol{x},t\,|\,\boldsymbol{x}',t')$ obeys the forward Fokker-Planck equation for a set of $\boldsymbol{x}$, t and $\boldsymbol{x}'$, t', and that the process is confined to a region R with boundary $\boldsymbol{S}$. Then, if s is a time between t and t',

$$0=\frac{\partial}{\partial s}p(\boldsymbol{x},t\,|\,\boldsymbol{x}',t')=\frac{\partial}{\partial s}\int d\boldsymbol{y}\,p(\boldsymbol{x},t\,|\,\boldsymbol{y},s)p(\boldsymbol{y},s\,|\,\boldsymbol{x}',t')\,, \tag{5.1.18}$$

where we have used the Chapman-Kolmogorov equation. We take the derivative $\partial/\partial s$ inside the integral, use the forward Fokker-Planck equation for the second factor and the backward equation for the first factor. For brevity, let us write

$$\left.\begin{aligned}p(\boldsymbol{y},s)&=p(\boldsymbol{y},s\,|\,\boldsymbol{x}',t')\,,\\ \bar{p}(\boldsymbol{y},s)&=p(\boldsymbol{x},t\,|\,\boldsymbol{y},s)\,.\end{aligned}\right\} \tag{5.1.19}$$

Then,

$$0=\int_R d\boldsymbol{y}\left[-\sum_i\frac{\partial}{\partial y_i}(A_ip)+\sum_{i,j}\frac{\partial^2}{\partial y_i\partial y_j}(B_{ij}p)\right]\bar{p}$$
$$+\int_R d\boldsymbol{y}\left[-\sum_i A_i\frac{\partial\bar{p}}{\partial y_i}-\sum_{i,j}B_{ij}\frac{\partial^2\bar{p}}{\partial y_i\partial y_j}\right]p\,, \tag{5.1.20}$$

and after some manipulation

$$=\int_R d\boldsymbol{y}\sum_i\frac{\partial}{\partial y_i}\left\{-A_ip\bar{p}+\frac{1}{2}\sum_j\left[\bar{p}\frac{\partial}{\partial y_j}(B_{ij}p)-pB_{ij}\frac{\partial\bar{p}}{\partial y_j}\right]\right\}\,, \tag{5.1.21}$$

$$=\int_S\sum_i dS_i\left\{\bar{p}\left[-A_ip+\frac{1}{2}\sum_j\frac{\partial}{\partial y_i}(B_{ij}p)\right]\right\}-\frac{1}{2}\int_S\sum_j dS_ip\left(\sum_j B_{ij}\frac{\partial\bar{p}}{\partial y_j}\right). \tag{5.1.22}$$

We now treat the various cases individually.

a) Absorbing Boundaries: This requires $p=0$ on the boundary. That it also requires $\bar{p}(\boldsymbol{y},t)=0$ on the boundary is easily seen to be consistent with (5.1.22) since on substituting $p=0$ in that equation, we get

$$0=\int_S\bar{p}\sum_{i,j}dS_iB_{ij}\frac{\partial p}{\partial y_j}\,. \tag{5.1.23}$$

However, if the boundary is absorbing, clearly

$$p(\boldsymbol{x},t\,|\,\boldsymbol{y},s)=0,\qquad \text{for}\quad \boldsymbol{y}\in\text{ boundary}, \tag{5.1.24}$$

since this merely states that the probability of X re-entering R from the boundary is zero.

b) Reflecting Boundaries: Here the condition on the forward equation makes the first integral vanish in (5.1.22). The final factor vanishes for arbitrary p only if

$$\sum_{i,j}n_iB_{ij}(\boldsymbol{y})\frac{\partial}{\partial y_j}[p(\boldsymbol{x},t\,|\,\boldsymbol{y},s)]=0\,. \tag{5.1.25}$$

In one dimension this reduces to

$$\frac{\partial}{\partial y}p(\boldsymbol{x},t\,|\,\boldsymbol{y},s)=0\,, \tag{5.1.26}$$

unless B vanishes.

c) Other Boundaries: We shall not consider these this section. For further details see [5.4].

5.2 Fokker-Planck Equation in One Dimension

In one dimension, the Fokker-Planck equation (FPE) takes the simple form

$$\frac{\partial f(x,t)}{\partial t}=-\frac{\partial}{\partial x}[A(x,t)f(x,t)]+\frac{1}{2}\frac{\partial^2}{\partial x^2}[B(x,t)f(x,t)]\,. \tag{5.2.1}$$

In Sects. 3.4, 3.5, the Fokker-Planck equation was shown to be valid for the conditional probability, that is, the choice

$$f(x,t) = p(x,t\,|\,x_0,t_0)\,, \tag{5.2.2}$$

for any initial x_0, t_0, and with the initial condition

$$p(x,t_0\,|\,x_0,t_0) = \delta(x-x_0)\,. \tag{5.2.3}$$

However, using the definition for the one time probability

$$p(x,t) = \int dx_0\, p(x,t;x_0,t_0) \equiv \int dx_0\, p(x,t\,|\,x_0,t_0)p(x_0,t_0)\,, \tag{5.2.4}$$

we see that it is also valid for $p(x,t)$ with the initial condition

$$p(x,t)|_{t=t_0} = p(x,t_0)\,, \tag{5.2.5}$$

which is generally less singular than (5.2.3).

From the result of Sect. 4.3.5, we know that the stochastic process described by a conditional probability satisfying the FPE is equivalent to the Ito stochastic differential equation (SDE)

$$dx(t) = A[x(t),t]\,dt + \sqrt{B[x(t),t]}\,dW(t)\,, \tag{5.2.6}$$

and that the two descriptions are to be regarded as complementary to each other. We will see that perturbation theories based on the FPE are very different from those based on the SDE and both have their uses.

5.2.1 Boundary Conditions in One Dimension

The general formulation of boundary conditions as given in Sect. 5.1.1 can be augmented by some more specific results for the one-dimensional case.

a) Periodic Boundary Condition: We assume that the process takes place on an interval $[a,b]$in which the two end points are identified with each other. (this occurs, for example, if the diffusion is on a circle). Then we impose boundary conditions derived from those for a discontinuity, i.e.,

$$\mathrm{I}: \lim_{x\to b-} p(x,t) = \lim_{x\to a+} p(x,t)\,, \tag{5.2.7}$$

$$\mathrm{II}: \lim_{x\to b-} J(x,t) = \lim_{x\to a+} J(x,t)\,. \tag{5.2.8}$$

Most frequently, periodic boundary conditions are imposed when the functions $A(x,t)$ and $B(x,t)$ are periodic on the same interval so that we have

$$\begin{aligned} A(b,t) &= A(a,t)\,,\\ B(b,t) &= B(a,t)\,, \end{aligned} \tag{5.2.9}$$

and this means that I and II simply reduce to an equality of $p(x,t)$ and its derivatives at the points a and b.

b) Prescribed Boundaries: If the diffusion coefficient vanishes at a boundary, we have a situation in which the kind of boundary may be automatically prescribed. Suppose the motion occurs only for $x > a$. If a Lipschitz condition is obeyed by $A(x,t)$ and $\sqrt{B(x,t)}$ at $x = a$ Sect. 4.3.1b) and $B(x,t)$ is differentiable at $x = a$ then

$$\partial_x B(a,t) = 0\,. \tag{5.2.10}$$

The SDE then has solutions, and we may write

$$dx(t) = A(x,t)dt + \sqrt{B(x,t)}\,dW(t)\,. \tag{5.2.11}$$

In this rather special case, the situation is determined by the sign of $A(x,t)$. Three cases then occur, as follows.

i) *Exit boundary*. In this case, we suppose

$$A(a,t) < 0\,, \tag{5.2.12}$$

so that if the particle reaches the point a, it will certainly proceed out of region to $x < a$. Hence the name "exit boundary"

ii) *Entrance boundary*. Suppose

$$A(a,t) > 0\,. \tag{5.2.13}$$

In this case, if the particle reaches the point a, the sign of $A(a,t)$ is such as to return it to $x > a$; thus a particle placed to the right of a can never leave the region. However, a particle introduced at $x = a$ will certainly enter the region. Hence the name, "entrance boundary".

iii) *Natural boundary*. Finally consider

$$A(a,t) = 0\,. \tag{5.2.14}$$

The particle, once it reaches $x = a$, will remain there. However it can be demonstrated that it cannot ever reach this point. This is a boundary from which we can neither absorb nor at which we can introduce any particles.

c) Feller's Classification of Boundaries: *Feller* [5.4] showed that in general the boundaries can be assigned to one of the four types; regular, entrance, exit and natural. His general criteria for the classification of these boundaries are as follows.

Define

$$f(x) = \exp\left[-2\int_{x_0}^{x} ds\, A(s)/B(s)\right], \tag{5.2.15}$$

$$g(x) = 2/[B(x)f(x)]\,, \tag{5.2.16}$$

$$h_1(x) = f(x)\int_{x_0}^{x} g(s)\,ds\,, \tag{5.2.17}$$

$$h_2(x) = g(x)\int_{x_0}^{x} f(s)\,ds\,. \tag{5.2.18}$$

Here $x_0 \in (a,b)$, and is fixed. Denote by

$$\mathscr{L}(x_1,x_2)\,, \tag{5.2.19}$$

the space of all functions integrable on the interval (x_1,x_2).

Then the boundary at a can be classified as

I:	Regular:	if $f(x) \in \mathscr{L}(a, x_0)$	and $g(x) \in \mathscr{L}(a, x_0)$
II:	Exit:	if $g(x) \notin \mathscr{L}(a, x_0)$	and $h_1(x) \in \mathscr{L}(a, x_0)$
III:	Entrance:	if $g(x) \in \mathscr{L}(a, x_0)$	and $h_2(x) \in \mathscr{L}(a, x_0)$
IV:	Natural:	all other cases.	

It can be seen from the results of Sect. 5.3 that for an exit boundary there is no normalisable stationary solution of the Fokker-Planck equation, and that the mean time to reach the boundary, (5.5.24), is finite. Similarly, if the boundary is exit, a stationary solution can exist, but the mean time to reach the boundary is infinite. In the case of a regular boundary, the mean time to reach the boundary is finite, but a stationary solution with a reflecting boundary at a does exist. The case of natural boundaries is harder to analyse. The reader is referred to [5.4] for a more complete description.

c) Boundaries at Infinity: All of the above kinds of boundary can occur at infinity, provided we can simultaneously guarantee the normalisation of the probability which, if $p(x)$ is reasonably well behaved, requires

$$\lim_{x\to\infty} p(x,t) = 0\,. \tag{5.2.20}$$

If $\partial_x p(x)$ is reasonably well behaved (i.e., does not oscillate infinitely rapidly as $x \to \infty$),

$$\lim_{x\to\infty} \partial_x p(x,t) = 0\,, \tag{5.2.21}$$

so that a nonzero current at infinity will usually require either $A(x,t)$ or $B(x,t)$ to become infinite there. Treatment of such cases is usually best carried out by changing to another variable which is finite at $x = \infty$.

Where there are boundaries at $x = \pm\infty$ and nonzero currents at infinity are permitted, we have two possibilities which do not allow for loss of probability:

$$\text{i)}\quad J(\pm\infty, t) = 0\,, \tag{5.2.22}$$

$$\text{ii)}\quad J(+\infty, t) = J(-\infty, t)\,. \tag{5.2.23}$$

These are the limits of reflecting and periodic boundary conditions, respectively.

5.3 Stationary Solutions for Homogeneous Fokker-Planck Equations

We recall (Sect. 3.7.2) that in a homogeneous process, the drift and diffusion coefficients are time independent. In such a case, the equation satisfied by the stationary distribution is

$$\frac{d}{dx}[A(x)p_s(x)] - \frac{1}{2}\frac{d^2}{dx^2}[B(x)p_s(x)] = 0\,, \tag{5.3.1}$$

which can also be written simply in terms of the current (as defined in Sect. 5.1)

$$\frac{dJ(x)}{dx} = 0\,, \tag{5.3.2}$$

which clearly has the solution

$$J(x) = \text{constant}\,. \tag{5.3.3}$$

Suppose the process takes place on an interval (a, b). Then we must have

$$J(a) = J(x) = J(b) \equiv J\,, \tag{5.3.4}$$

and if one of the boundary conditions is reflecting, this means that both are reflecting, and $J = 0$.

If the boundaries are not reflecting, (5.3.4) requires them to be periodic. We then use the boundary conditions given by (5.2.7) and (5.2.8).

a) Zero Current—Potential Solution:

Setting $J = 0$, we rewrite (5.3.4) as

$$A(x)p_s(x) = \frac{1}{2}\frac{d}{dx}[B(x)p_s(x)] = 0\,, \tag{5.3.5}$$

for which the solution is

$$p_s(x) = \frac{\mathscr{N}}{B(x)} \exp\left[2\int_a^x dx' A(x')/B(x')\right], \tag{5.3.6}$$

where $\mathscr{N}$ is a normalisation constant such that

$$\int_a^b dx\, p_s(x) = 1\,. \tag{5.3.7}$$

Such a solution is known as a *potential solution*, for various historical reasons, but chiefly because the stationary solution is obtained by a single integration (the full significance of this term will be treated in Sect. 6.2.2).

b) Periodic Boundary Condition: Here we have nonzero current J and we rewrite (5.3.3) as

$$A(x)p_s(x) - \frac{1}{2}\frac{d}{dx}[B(x)p_s(x)] = J\,. \tag{5.3.8}$$

However, J is not arbitrary, but is determined by normalisation and the periodic boundary condition

$$p_s(a) = p_s(b)\,, \tag{5.3.9}$$

$$J(a) = J(b)\,. \tag{5.3.10}$$

For convenience, define

$$\psi(x) = \exp\left[2\int_a^x dx' A(x')/B(x')\right]. \tag{5.3.11}$$

Then we can easily integrate (5.3.8) to get

$$\frac{p_s(x)B(x)}{\psi(x)} = \frac{p_s(a)B(a)}{\psi(a)} - 2J\int_a^x \frac{dx'}{\psi(x')}\,. \tag{5.3.12}$$

By imposing the boundary condition (5.3.9) we find that

$$J = \frac{\left[\frac{B(b)}{\psi(b)} - \frac{B(a)}{\psi(a)}\right] p_s(a)}{\int_a^b \frac{dx'}{\psi(x')}}, \tag{5.3.13}$$

so that

$$p_s(x) = p_s(a)\left[\frac{\int_a^x \frac{dx'}{\psi(x')}\frac{B(b)}{\psi(b)} + \int_x^b \frac{dx'}{\psi(x')}\frac{B(a)}{\psi(a)}}{\frac{B(x)}{\psi(x)}\int_a^b \frac{dx'}{\psi(x')}}\right]. \tag{5.3.14}$$

c) Infinite Range and Singular Boundaries: In either of these cases, one or the other of the above possibilities may turn out to be forbidden because of divergences, etc. A full enumeration of the possibilities is, in general, very complicated. We shall demonstrate these by means of the examples given in the next section.

5.3.1 Examples of Stationary Solutions

a) Diffusion in a Gravitational Field: A strongly damped Brownian particle moving in a constant gravitational field is often described by the stochastic differential equation (8.2.15)

$$dx = -g\,dt + \sqrt{D}\,dW(t), \tag{5.3.15}$$

for which the Fokker-Planck equation is

$$\frac{\partial p}{\partial t} = \frac{\partial}{\partial x}(gp) + \frac{1}{2}D\frac{\partial^2 p}{\partial x^2}. \tag{5.3.16}$$

On the interval (a, b) with reflecting boundary conditions, the stationary solution is given by (5.3.6), i.e.

$$p_s(x) = \mathcal{N} \exp[-2gx/D], \tag{5.3.17}$$

where we have absorbed constant factors into the definition of $\mathcal{N}$.

Clearly this solution is normalisable on (a, b) only if a a is finite, though b may be infinite. The result is no more profound than to say that particles diffusing in a beaker of fluid will fall down, and if the beaker is infinitely deep, they will never stop falling! Diffusion upwards against gravity is possible for any distance but with exponentially small probability.

Now assume periodic boundary conditions on (a, b). Substitution into (5.3.14) yields

$$p_s(x) = p_s(a), \tag{5.3.18}$$

a constant distribution.

The interpretation is that the particles pass freely from a to b and back.

b) Ornstein Uhlenbeck Process: We use the notation of Sect. 3.8.4 where the Fokker-Planck equation was

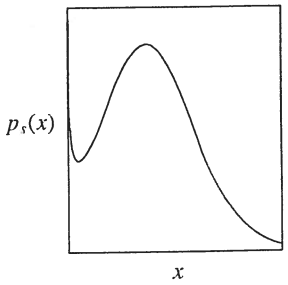

Fig. 5.2. Non-normalisable "stationary" $p_s(x)$ for the reaction $X + A \rightleftharpoons 2X$.

$$\frac{\partial p}{\partial t} = \frac{\partial}{\partial x}(kxp) + \frac{1}{2}D\frac{\partial^2 p}{\partial x^2}, \tag{5.3.19}$$

whose stationary solution on the interval (a, b) with reflecting barriers is

$$p_s(x) = \mathcal{N} \exp(-kx^2/D). \tag{5.3.20}$$

Provided $k > 0$, this is normalisable on $(-\infty, \infty)$.

If $k < 0$, one can only make sense of it on a finite interval. In this case suppose

$$a = -b < 0. \tag{5.3.21}$$

so that from (5.3.11),

$$\psi(x) = \exp\left[-\frac{k}{D}(x^2 - a^2)\right], \tag{5.3.22}$$

and if we consider the periodic boundary condition on this interval, by noting

$$\psi(a) = \psi(-a), \tag{5.3.23}$$

we find that

$$p_s(x) = p_s(a)\frac{\psi(x)}{\psi(a)} = p_s(a)\exp\left[-\frac{k}{D}(x^2 - a^2)\right], \tag{5.3.24}$$

so that the symmetry yields the same solution as in the case of reflecting barriers.

Letting $a \to \infty$, we see that we still have the same solution. The result is also true if $a \to \infty$ independently of $b \to -\infty$, provided $k > 0$.

c) A Chemical Reaction Model: Although chemical reactions are normally best modelled by a birth-death master equation formalism, as in Chap. 11, approximate treatments are often given by means of a Fokker-Planck equation. The reaction

$$X + A \rightleftharpoons 2X, \tag{5.3.25}$$

is of interest since it possesses an exit boundary at $x = 0$ (where x is the number of molecules of X). Clearly if there is no X, a collision between X and A cannot occur so no more X is produced.

The Fokker-Planck equation is derived in Sect. 11.6.1 and is

$$\partial_t p(x,t) = -\partial_x\left[\left(ax - x^2\right)p(x,t)\right] + \tfrac{1}{2}\partial_x^2\left[\left(ax + x^2\right)p(x,t)\right]. \tag{5.3.26}$$

We introduce reflecting boundaries at $x = \alpha$ and $x = \beta$. In this case, the stationary solution is

$$p_s(x) = e^{-2x}(a+x)^{4a-1}x^{-1}, \tag{5.3.27}$$

which is not normalisable if $\alpha = 0$. The pole at $x = 0$ is a result of the absorption there. In fact, comparing with (5.2.18), we see that

$$\left.\begin{aligned} B(0,t) &\equiv (ax + x^2)_{x=0} = 0, \\ A(0,t) &\equiv (ax - x^2)_{x=0} = 0, \\ \partial_x B(0,t) &\equiv (a+2x)_{x=0} > 0, \end{aligned}\right\} \tag{5.3.28}$$

so we indeed have an exit boundary. The stationary solution has relevance only if $\alpha > 0$ since it is otherwise not normalisable. The physical meaning of a reflecting barrier is quite simple: whenever a molecule of X disappears, we simply add another one immediately. A plot of $p_s(x)$ is given in Fig. 5.2. The time for all x to disappear is in practice extraordinarily long, and the stationary solution (5.3.27) is, in practice, a good representation of the distribution except near $x = 0$.

5.4 Eigenfunction Methods for Homogeneous Processes

We shall now show how, in the case of homogeneous processes, solutions can most naturally be expressed in terms of eigenfunctions. We consider reflecting and absorbing boundaries.

5.4.1 Eigenfunctions for Reflecting Boundaries

We consider a Fokker-Planck equation for a process on a interval (a, b) with reflecting boundaries. We suppose the Fokker-Planck equation to have a stationary solution $p_s(x)$ and the from

$$\partial_t p(x,t) = -\partial_x[A(x)p(x,t)] + \tfrac{1}{2}\partial_x^2[B(x)p(x,t)]. \tag{5.4.1}$$

We define a function $q(x,t)$ by

$$p(x,t) = p_s(x)q(x,t), \tag{5.4.2}$$

and, by direct substitution, find that $q(x,t)$ satisfies the *backward equation*

$$\partial_t q(x,t) = A(x)\partial_x q(x,t) + \tfrac{1}{2}B(x)\partial_x^2 q(x,t). \tag{5.4.3}$$

We now wish to consider solutions of the form

$$p(x,t) = P_\lambda(x)e^{-\lambda t}, \tag{5.4.4}$$

$$q(x,t) = Q_\lambda(x)e^{-\lambda t}, \tag{5.4.5}$$

which obey the eigenfunction equations

$$-\partial_x[A(x)P_\lambda(x)] + \tfrac{1}{2}\partial_x^2[B(x)P_\lambda(x)] = -\lambda P_\lambda(x), \tag{5.4.6}$$

$$A(x)\partial_x Q_{\lambda'}(x) + \tfrac{1}{2}B(x)\partial_x^2 Q_{\lambda'}(x) = -\lambda' Q_{\lambda'}(x). \tag{5.4.7}$$

i) *Relationship between P_λ and Q_λ :* From (5.4.2) and (5.4.3) it follows that

$$P_\lambda(x) = p_s(x)Q_\lambda(x). \tag{5.4.8}$$

This simple result does not generalise completely to many dimensional situations, which are treated in Sect. 6.5.

ii) *Orthogonality of eigenfunctions:* We can straightforwardly show by partial integration that

$$\begin{aligned}(\lambda' - \lambda)\int_a^b dx P_\lambda(x)Q_{\lambda'}(x) \\ = \left[Q_{\lambda'}(x)\left\{-A(x)P_\lambda(x) + \tfrac{1}{2}\partial_x[B(x)P_\lambda(x)]\right\} - \tfrac{1}{2}B(x)P_\lambda(x)\partial_x Q_{\lambda'}(x)\right]_a^b.\end{aligned} \tag{5.4.9}$$

Using the reflecting boundary condition on the coefficient of $Q_{\lambda'}(x)$, we see that this coefficient vanishes. Further, using the definition of $q(x,t)$ in terms of the stationary solution (5.4.2), it is simple to show that

$$\tfrac{1}{2}B(x)\partial_x Q_{\lambda'}(x) = -A(x)P_{\lambda'}(x) + \tfrac{1}{2}\partial_x[B(x)P_{\lambda'}(x)], \tag{5.4.10}$$

so that term vanishes also. Hence, the $Q_\lambda(x)$ and $P_\lambda(x)$ form a bi-orthogonal system

$$\int_a^b dx\, P_\lambda(x)Q_{\lambda'}(x) = \delta_{\lambda\lambda'}. \tag{5.4.11}$$

There are thus are two alternative *orthogonality* systems,

$$\int_a^b dx\, p_s(x)Q_\lambda(x)Q_{\lambda'}(x) = \delta_{\lambda\lambda'}, \tag{5.4.12}$$

$$\int_a^b dx [p_s(x)]^{-1}P_\lambda(x)P_{\lambda'}(x) = \delta_{\lambda\lambda'}. \tag{5.4.13}$$

It should be noted that setting $\lambda = \lambda' = 0$ gives the normalisation of the stationary solution $p_s(x)$ since

$$P_0(x) = p_s(x), \tag{5.4.14}$$

$$Q_0(x) = 1. \tag{5.4.15}$$

iii) *Expansion in eigenfunctions:* Using this orthogonality (and assuming completeness) we can write any solution in terms of eigenfunctions. For if

$$p(x,t) = \sum_\lambda A_\lambda P_\lambda(x)e^{-\lambda t}, \tag{5.4.16}$$

then

$$\int_a^b dx\, Q_\lambda(x)p(x,0) = A_\lambda. \tag{5.4.17}$$

iv) *Conditional probability:* For example, the conditional probability $p(x,t\,|\,x_0,0)$ is given by the initial condition

$$p(x,0\,|\,x_0,0)=\delta(x-x_0)\,, \tag{5.4.18}$$

so that

$$A_\lambda=\int_a^b dx\,Q_\lambda(x)\delta(x-x_0)=Q_\lambda(x_0)\,, \tag{5.4.19}$$

and hence,

$$p(x,t\,|\,x_0,0)=\sum_\lambda P_\lambda(x)Q_\lambda(x_0)\mathrm{e}^{-\lambda t}\,. \tag{5.4.20}$$

v) *Autocorrelation function:* We can write the autocorrelation function quite elegantly as

$$\langle x(t)x(0)\rangle=\int dx\int dx_0\,x\,x_0\,p(x,t\,|\,x_0,0)p_s(x)\,, \tag{5.4.21}$$

$$=\sum_\lambda\left[\int dx\,xP_\lambda(x)\right]^2\mathrm{e}^{-\lambda t}\,, \tag{5.4.22}$$

where we have used the definition of $Q_\lambda(x)$ by (5.4.5).

5.4.2 Eigenfunctions for Absorbing Boundaries

These are treated similarly.

We define P_λ and Q_λ as above, except that $p_s(x)$ is still the stationary solution of the Fokker-Planck equation with *reflecting boundary conditions*. With this definition, we find that we must have

$$P_\lambda(a)=Q_\lambda(a)=P_\lambda(b)=Q_\lambda(b)=0\,, \tag{5.4.23}$$

and the orthogonality proof still follows through. Eigenfunctions are then computed using this condition and the eigenfunction equations (5.4.6) and (5.4.7) and all other results look the same. However, the range of λ does not include $\lambda=0$, and hence $p(x,t\,|\,x_0,0)\to 0$ as $t\to\infty$.

5.4.3 Examples

a) A Wiener Process with Absorbing Boundaries: The Fokker-Planck equation

$$\partial_t p=\tfrac{1}{2}\partial_x^2 p\,, \tag{5.4.24}$$

is treated on the interval $(0,1)$. The absorbing boundary condition requires

$$p(0,t)=p(1,t)=0\,, \tag{5.4.25}$$

and the appropriate eigenfunctions are $\sin(n\pi x)$ so we expand in a Fourier sine series

$$p(x,t)=\sum_{n=1}^\infty b_n(t)\sin(n\pi x)\,, \tag{5.4.26}$$

which automatically satisfies (5.4.25). The initial condition is chosen so that

$$p(x,0)=\delta(x-x_0)\,, \tag{5.4.27}$$

for which the Fourier coefficients are

$$b_n(0)=2\int_0^1 dx\,\delta(x-x_0)\sin(n\pi x)=2\sin(n\pi x_0)\,. \tag{5.4.28}$$

Substituting the Fourier expansion (5.4.26) into (5.4.24) gives

$$\frac{db_n(t)}{dt}=-\lambda_n b_n(t)\,, \tag{5.4.29}$$

with

$$\lambda_n=n^2\pi^2/2\,, \tag{5.4.30}$$

and the solution

$$b_n(t)=b_n(0)\exp(-\lambda_n t)\,. \tag{5.4.31}$$

So we have the solution [which by the initial condition (5.4.27) is for the conditional probability $p(x,t\,|\,x_0,0)$]

$$p(x,t\,|\,x_0,0)=2\sum_{n=1}^\infty\exp(-\lambda_n t)\sin(n\pi x_0)\sin(n\pi x)\,. \tag{5.4.32}$$

b) Wiener Process with Reflecting Boundaries: Here the boundary condition reduces to [on the interval $(0,1)$]

$$\partial_x p(0,t)=\partial_x p(1,t)=0\,, \tag{5.4.33}$$

and the eigenfunctions are now $\cos(n\pi x)$, so we make a Fourier cosine expansion

$$p(x,t)=\tfrac{1}{2}a_0+\sum_{n=1}^\infty a_n(t)\cos(n\pi x)\,, \tag{5.4.34}$$

with the same initial condition

$$p(x,0)=\delta(x-x_0)\,, \tag{5.4.35}$$

so that

$$a_n(0)=2\int_0^1 dx\,\cos(n\pi x)\delta(x-x_0)=2\cos(n\pi x_0)\,. \tag{5.4.36}$$

In the same way as before, we find

$$a_n(t)=a_n(0)\exp(-\lambda_n t)\,, \tag{5.4.37}$$

with

$$\lambda_n=n^2\pi^2/2\,, \tag{5.4.38}$$

so that

$$p(x,t\,|\,x_0,0)=1+2\sum_{n=1}^\infty\cos(n\pi x_0)\cos(n\pi x)\exp(-\lambda_n t)\,. \tag{5.4.39}$$

As $t\to\infty$, the process becomes stationary, with stationary distribution

$$p_s(x) = \lim_{t\to\infty} p(x,t\,|\,x_0,0) = 1. \tag{5.4.40}$$

We can compute the stationary autocorrelation function by

$$\langle x(t)x(0)\rangle_s = \int_0^1\int_0^1 dx\,dx_0\,x\,x_0\,p(x,t\,|\,x_0,0)p_s(x)\,, \tag{5.4.41}$$

and carrying out the integrals explicitly,

$$\langle x(t)x(0)\rangle_s = \frac{1}{4} + \frac{8}{\pi^4}\sum_{n=0}^{\infty}\exp(-\lambda_{2n+1}t)(2n+1)^{-4}\,. \tag{5.4.42}$$

We see that as $t\to\infty$, all the exponentials vanish and

$$\langle x(t)x(0)\rangle_s \to \frac{1}{4} = [\langle x\rangle_s]^2\,, \tag{5.4.43}$$

and as $t\to 0$,

$$\langle x(t)x(0)\rangle_s \to \frac{1}{4} + \frac{8}{\pi^4}\sum_{n=0}^{\infty}(2n+1)^{-4} = \frac{1}{3} = \langle x_s^2\rangle\,, \tag{5.4.44}$$

when one takes account of the identity (from the theory of the Riemann zeta-function)

$$\sum_{n=0}^{\infty}(2n+1)^{-4} = \frac{\pi^4}{96}\,. \tag{5.4.45}$$

c) Ornstein-Uhlenbeck Process: As in Sect. 3.8.4 the Fokker-Planck equation is

$$\partial_t p(x,t) = \partial_x[kxp(x,t)] + \tfrac{1}{2}D\partial_x^2 p(x,t)\,. \tag{5.4.46}$$

The eigenfunction equation for Q_λ is

$$d_x^2 Q_\lambda - \frac{2kx}{d}d_x Q_\lambda + \frac{2\lambda}{D}Q_\lambda = 0\,, \tag{5.4.47}$$

and this becomes the differential equation for *Hermite polynomials* $\mathrm{H}_n(y)$ [5.5] on making the replacement $y = x\sqrt{k/D}$:

$$d_y^2 Q_\lambda - 2yd_y Q_\lambda + (2\lambda/k)Q_\lambda = 0\,. \tag{5.4.48}$$

We can write

$$Q_\lambda = (2^n n!)^{-1/2}\mathrm{H}_n\left(x\sqrt{k/D}\right)\,, \tag{5.4.49}$$

where

$$\lambda = nk\,, \tag{5.4.50}$$

and these solutions are normalised as in (5.4.11–5.4.13).

The stationary solution is, as previously found,

$$p_s(x) = (k/\pi D)^{1/2}\exp(-kx^2/D)\,, \tag{5.4.51}$$

and a general solution can be written as

$$p(x,t) = \sum_n \sqrt{[k/(2^n n!\pi D)]}\exp(-kx^2/D)\mathrm{H}_n\left(x\sqrt{k/D}\right)\mathrm{e}^{-nkt}A_n\,, \tag{5.4.52}$$

with

$$A_n = \int_{-\infty}^{\infty} dx\,p(x,0)\mathrm{H}_n\left(x\sqrt{k/D}\right)(2^n n!)^{-1/2}\,. \tag{5.4.53}$$

The result can also be obtained directly from the explicit solution for the conditional probability given in Sect. 3.8.4 by using generating functions for Hermite polynomials. One sees that the time scale of relaxation to the stationary state is given by the eigenvalues

$$\lambda_n = nk\,. \tag{5.4.54}$$

Here, k is the rate constant for deterministic relaxation, and it thus determines the slowest time in the relaxation. One can also compute the autocorrelation function directly using (5.4.22). We use the result [5.5] that

$$\mathrm{H}_1(y) = 2y\,, \tag{5.4.55}$$

so that the orthogonality property means that only the eigenfunction corresponding to $n = 1$ has a nonzero coefficient. We must compute

$$\int xP_{\lambda_1}(x)dx = \int_{-\infty}^{\infty} dx\,\sqrt{k/(2\pi D)}\exp(-kx^2/D)\left(2x\sqrt{k/D}\right)x = \sqrt{D/2k}\,, \tag{5.4.56}$$

so that

$$\langle x(t)x(0)\rangle_s = \frac{D}{2k}\mathrm{e}^{-kt}\,, \tag{5.4.57}$$

as found previously in Sects. 3.8.4 and 4.5.4.

d) Rayleigh Process: We take the model of amplitude fluctuations developed in Sect. 4.5.5. The Fokker-Planck equation is

$$\partial_t p(x,t) = \partial_x[(\gamma x - \mu/x)p(x,t)] + \mu\partial_x^2 p(x,t)\,, \tag{5.4.58}$$

where

$$\mu = \varepsilon^2/2\,. \tag{5.4.59}$$

The range here is $(0,\infty)$ and the stationary solution (normalised)

$$p_s(x) = (\gamma x/\mu)\exp(-\gamma x^2/2\mu)\,. \tag{5.4.60}$$

The eigenfunction equation for the $Q_\lambda(x)$ is

$$d_x^2 Q_\lambda + (1/x - \gamma x/\mu)d_x Q_\lambda + (\lambda/\mu)Q_\lambda = 0\,. \tag{5.4.61}$$

By setting

$$z = x^2\gamma/2\mu\,, \tag{5.4.62}$$

we obtain

$$zd_z^2 Q_\lambda + (1-z)d_z Q_\lambda + (\lambda/2\gamma)Q_\lambda = 0\,. \tag{5.4.63}$$

This is the differential equation for the *Laguerre polynomials* $\mathrm{L}_n(y)$ [5.5] provided

$$\lambda = 2n\gamma\,. \tag{5.4.64}$$

We can write

$$Q_\lambda(x) = \mathrm{L}_n(\gamma x^2/2\mu)\,, \tag{5.4.65}$$

which is normalised. Hence, the conditional probability is

$$p(x,t\,|\,x_0,0) = \sum_{n=0}^{\infty} \frac{\gamma x}{\mu} \exp\left(-\frac{\gamma x^2}{2\mu}\right) \mathrm{L}_n\left(\frac{\gamma x_0^2}{2\mu}\right) \mathrm{L}_n\left(\frac{\gamma x^2}{2\mu}\right) \mathrm{e}^{-2n\gamma t}\,. \tag{5.4.66}$$

We can compute the autocorrelation function by the method of (5.4.22):

$$\langle x(t)x(0)\rangle = \sum_{n=0}^{\infty} \left[\int_0^{\infty} x\,dx \frac{\gamma x}{\mu} \exp\left(\frac{-\gamma x^2}{2\mu}\right) \mathrm{L}_n\left(\frac{\gamma x^2}{2\mu}\right)\right]^2 \exp(-2n\gamma t)\,, \tag{5.4.67}$$

and using

$$\int_0^{\infty} dz\, z^{\alpha} \mathrm{e}^{-z} \mathrm{L}_n(z) = (-1)^n \Gamma(\alpha+1) \binom{\alpha}{n}, \tag{5.4.68}$$

we find for the autocorrelation function

$$\langle x(t)x(0)\rangle = \frac{2\mu}{\gamma} \sum_{n=0}^{\infty} \frac{\pi}{4} \binom{\frac{1}{2}}{n}^2 \exp(-2n\gamma t)\,. \tag{5.4.69}$$

5.5 First Passage Times for Homogeneous Processes

It is often of interest to know how long a particle whose position is described by a Fokker-Planck equation remains in a certain region of x. The solution of this problem can be achieved by use of the *backward Fokker-Planck equation*, as described in Sect. 3.6.

5.5.1 Two Absorbing Barriers

Let the particle be initially at x at time $t = 0$ and let us ask how long it remains in the interval (a, b) which is assumed to contain x:

$$a \leqslant x \leqslant b\,. \tag{5.5.1}$$

We erect absorbing barriers at a and b so that the particle is removed from the system when it reaches a or b. Hence, if it is still in the interval (a, b), it has never left that interval.

i) *Distribution of exit times:* Under these conditions, the probability that at time t the particle is still in (a, b) is

$$\int_a^b dx'\, p(x',t\,|\,x,0) \equiv G(x,t)\,. \tag{5.5.2}$$

Let the time that the particle leaves (a, b) be T. Then we can rewrite (5.5.2) as

$$\mathrm{Prob}(T \geqslant t) = \int_a^b dx'\, p(x',t\,|\,x,0)\,, \tag{5.5.3}$$

which means that $G(x,t)$ is the same as $\mathrm{Prob}(T \geqslant t)$. Since the system is time homogeneous, we can write

$$p(x',t\,|\,x,0) = p(x',0\,|\,x,-t)\,, \tag{5.5.4}$$

and the backward Fokker-Planck equation can be written

$$\partial_t p(x',t\,|\,x,0) = A(x)\partial_x p(x',t\,|\,x,0) + \tfrac{1}{2}B(x)\partial_x^2 p(x',t\,|\,x,0)\,, \tag{5.5.5}$$

and hence, $G(x,t)$ obeys the equation

$$\partial_t G(x,t) = A(x)\partial_x G(x,t) + \tfrac{1}{2}B(x)\partial_x^2 G(x,t)\,. \tag{5.5.6}$$

ii) *Initial condition:* Clearly that

$$p(x',0\,|\,x,0) = \delta(x-x')\,, \tag{5.5.7}$$

and hence,

$$G(x,0) = \begin{cases} 1\,, & a \leqslant x \leqslant b, \\ 0\,. & \text{elsewhere.} \end{cases} \tag{5.5.8}$$

iii) *Boundary conditions:* If $x = a$ or b, the particle is absorbed immediately, so $\mathrm{Prob}(T \geqslant t) = 0$ when $x = a$ or $x = b$, i.e.,

$$G(a,t) = G(b,t) = 0\,. \tag{5.5.9}$$

iv) *Moments of the exit time:* Since $G(x,t)$ is the probability that $T \geqslant t$, the mean of any function of T is

$$\langle f(T)\rangle = -\int_0^{\infty} f(t)\, dG(x,t)\,. \tag{5.5.10}$$

Thus, the *mean exit time* (or *mean first passage time*)

$$T(x) = \langle T\rangle\,, \tag{5.5.11}$$

is given by

$$T(x) = -\int_0^{\infty} t\,\partial_t G(x,t)dt \tag{5.5.12}$$

$$= \int_0^{\infty} G(x,t)dt\,, \tag{5.5.13}$$

after integrating by parts. Similarly, defining

$$T_n(x) = \langle T^n\rangle\,, \tag{5.5.14}$$

we find

$$T_n(x) = \int_0^{\infty} t^{n-1} G(x,t)dt\,. \tag{5.5.15}$$

v) *Differential equation for the mean exit time:* We can derive a simple ordinary differential equation for $T(x)$ by using (5.5.13) and integrating (5.5.6) over $(0, \infty)$. Noting that

$$\int_0^\infty \partial_t G(x,t)dt = G(x,\infty) - G(x,0) = -1\,, \tag{5.5.16}$$

we derive

$$A(x)\partial_x T(x) + \tfrac{1}{2}B(x)\partial_x^2 T(x) = -1\,, \tag{5.5.17}$$

with the boundary condition

$$T(a) = T(b) = 0\,. \tag{5.5.18}$$

Similarly, we see that

$$-nT_{n-1}(x) = A(x)\partial_x T_n(x) + \tfrac{1}{2}B(x)\partial_x^2 T_n(x)\,. \tag{5.5.19}$$

vi) *Solutions of the Equations:* Equation (5.5.17) can be solved directly by integration. The solution, after some manipulation, can be written in terms of

$$\psi(x) = \exp\left\{\int_0^x dx'[2A(x')/B(x')]\right\}. \tag{5.5.20}$$

We find

$$T(x) = \frac{2\left[\left(\int_a^x \frac{dy}{\psi(y)}\right)\int_x^b \frac{dy'}{\psi(y')}\int_a^{y'}\frac{dz\,\psi(z)}{B(z)} - \left(\int_x^b \frac{dy}{\psi(y)}\right)\int_a^x \frac{dy'}{\psi(y')}\int_a^{y'}\frac{dz\,\psi(z)}{B(z)}\right]}{\int_a^b \frac{dy}{\psi(y)}}\,. \tag{5.5.21}$$

5.5.2 One Absorbing Barrier

We consider motion still in the interval (a,b) but suppose the barrier at a to be reflecting. The boundary conditions then become

$$\partial_x G(a,t) = 0\,, \tag{5.5.22a}$$

$$G(b,t) = 0\,, \tag{5.5.22b}$$

which follow from the conditions on the backward Fokker-Planck equation derived in Sect. 5.1.2. We solve (5.5.17) with the corresponding boundary condition and obtain

$$T(x) = 2\int_x^b \frac{dy}{\psi(y)}\int_a^y \frac{\psi(z)}{B(z)}dz \qquad \begin{array}{l} a \text{ reflecting,} \\ b \text{ absorbing,} \\ a < b\,. \end{array} \tag{5.5.23}$$

Similarly, one finds

$$T(x) = 2\int_a^x \frac{dy}{\psi(y)}\int_y^b \frac{\psi(z)}{B(z)}dz \qquad \begin{array}{l} b \text{ reflecting,} \\ a \text{ absorbing,} \\ a < b\,. \end{array} \tag{5.5.24}$$

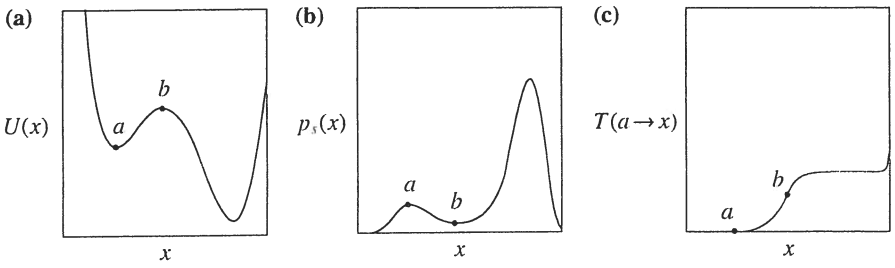

Fig. 5.3. (**a**) Double well potential $U(x)$; (**b**) Stationary distribution $p_s(x)$; (**c**) Mean first passage time from a to x, $T(a \to x)$

5.5.3 Application—Escape Over a Potential Barrier

We suppose that a point moves according to the Fokker-Planck equation

$$\partial_t p(x,t) = \partial_x[U'(x)p(x,t)] + D\partial_x^2 p(x,t)\,. \tag{5.5.25}$$

The potential has maxima and minima, as shown in Fig. 5.3. We suppose that motion is on an infinite range, which means the stationary solution is

$$p_s(x) = \mathcal{N}\exp[-U(x)/D]\,, \tag{5.5.26}$$

which is bimodal (as shown in Fig. 5.3) so that there is a relatively high probability of being on the left or the right of b, but not near b. What is the mean escape time from the left hand well? By this we mean, what is the mean first passage time from a to x, where x is in the vicinity of b? We use (5.5.23) with the substitutions

$$b \to x, \quad a \to -\infty, \quad x \to a\,, \tag{5.5.27}$$

so that

$$T(a \to x) = \frac{1}{D}\int_a^x dy\exp[U(y)/D]\int_{-\infty}^y \exp[-U(z)/D]dz\,. \tag{5.5.28}$$

If the central maximum of $U(x)$ is large and D is small, then $\exp[U(y)/D]$ is sharply peaked at $x = b$, while $\exp[-U(z)/D]$ is very small near $z = b$. Therefore, $\int_{-\infty}^y \exp[-U(z)/D]dz$ is a very slowly varying function of y near $y = b$. This means that the value of the integral $\int_{-\infty}^y \exp[-U(z)/D]dz$ will be approximately constant for those values of y which yield a value of $\exp[U(y)/D]$ which is significantly different from zero. Hence, in the inner integral, we can set $y = b$ and remove the resulting constant factor from inside the integral with respect to y. Thus, we can approximate (5.5.28) by

$$T(a \to x) \approx \left\{\frac{1}{D}\int_{-\infty}^b dy\exp[-U(z)/D]\right\}\int_a^x dy\exp[U(y)/D]\,. \tag{5.5.29}$$

Notice that by the definition of $p_s(x)$ in (5.5.26), we can say that

$$\int_{-\infty}^b dy\exp[-U(z)/D] = n_a/\mathcal{N}\,, \tag{5.5.30}$$

which means that n_a is the probability that the particle is to the left of b when the system is stationary.

A plot of $T(a \to x_0)$ against x_0 is shown in Fig. 5.3 and shows that the mean first passage time to x_0 is quite small for x_0 in the left well and quite large for x_0 in the right well. This means that the particle, in going over the barrier to the right well, takes most of the time in actually surmounting the barrier. It is quite meaningful to talk of the *escape time* as that time for the particle, initially at a, to reach a point near c, since this time is quite insensitive to the exact location of the initial and final points. We can evaluate this by further assuming that near b we can write

$$U(x) \approx U(b) - \tfrac{1}{2}\left(\frac{x-b}{\delta}\right)^2, \tag{5.5.31}$$

and near a

$$U(x) \approx U(a) + \tfrac{1}{2}\left(\frac{x-a}{\alpha}\right)^2. \tag{5.5.32}$$

The constant factor in (5.5.29) is evaluated as

$$\int_{-\infty}^{b} dz \exp[-U(z)/D] \approx \int_{-\infty}^{\infty} dz \exp\left[-\frac{U(a)}{D} - \frac{(z-a)^2}{2D\alpha^2}\right], \tag{5.5.33}$$

$$\approx \alpha\sqrt{2\pi D}\exp[-U(a)/D], \tag{5.5.34}$$

and the inner factor becomes, on assuming x_0 is well to the right of the central point b,

$$\int_{a}^{x} dy \exp U(y)/D] \approx \int_{-\infty}^{\infty} dy \exp\left[\frac{U(b)}{D} - \frac{(y-b)^2}{2D\delta^2}\right], \tag{5.5.35}$$

$$= \delta\sqrt{2\pi D}\exp[U(b)/D]. \tag{5.5.36}$$

Putting both of these in (5.5.29), we get

$$T(a \to x) \approx 2\alpha\delta\pi \exp\{[U(b) - U(a)]/D\}. \tag{5.5.37}$$

This is the classical *Arrhenius formula* of chemical reaction theory. In a chemical reaction, we can model the reaction by introducing a coordinate such that $x = a$ is species A and $x = c$ is species C. The reaction is modelled by the above diffusion process and the two distinct chemical species are separated by the potential barrier at b. In the chemical reaction, statistical mechanics gives the value

$$D = kT, \tag{5.5.38}$$

where k is Boltzmann's constant and T is the absolute temperature. We see that the most important dependence on temperature comes from the exponential factor which is often written

$$\exp(\Delta E/kT), \tag{5.5.39}$$

and predicts a very characteristic dependence on temperature. Intuitively, the answer is obvious. The exponential factor represents the probability that the energy will exceed that of the barrier when the system is in thermal equilibrium. Those molecules that reach this energy then react, with a certain finite probability.

We will come back to problems like this in great detail in Chap. 14.

5.5.4 Probability of Exit Through a Particular End of the Interval

What is the probability that the particle, initially at x in (a,b) exits through a, and what is the mean exit time?

The total probability that the particle exits through a after time t is given by the time integral of the probability current at a. We thus define this probability by

$$g_a(x,t) = -\int_t^{\infty} dt'\, J(a,t' \mid x,0), \tag{5.5.40}$$

$$= \int_t^{\infty} dt' \left\{-A(a)p(a,t' \mid x,0) + \tfrac{1}{2}\partial_a[B(a)p(a,t' \mid x,0)]\right\}. \tag{5.5.41}$$

the negative sign being chosen since we need the current pointing to the left. Similarly we define

$$g_b(x,t) = \int_t^{\infty} dt' \left\{A(b)p(b,t' \mid x,0) - \tfrac{1}{2}\partial_b[B(b)p(b,t' \mid x,0)]\right\}. \tag{5.5.42}$$

These two quantities give the probabilities that the particle exits through a or b after time t, respectively. The probability that (given that it exits through a) it exits after time t is

$$\text{Prob}(T_a > t) = g_a(x,t)/g_a(x,0). \tag{5.5.43}$$

We now find an equation for $g_a(x,t)$, using the fact that $p(a,t \mid x,0)$ satisfies a backward Fokker-Planck equation. Thus,

$$A(x)\partial_x g_a(x,t) + \tfrac{1}{2}B(x)\partial_x^2 g_a(x,t) = -\int_t^{\infty} dt' \partial_{t'} J(a,t' \mid x,0),$$

$$= J(a,t \mid x,0),$$

$$= \partial_t g_a(x,t). \tag{5.5.44}$$

The mean exit time, given that exit is through a, is

$$T(a,x) = -\int_0^{\infty} t\,\partial_t \text{Prob}\,(T_a > t)\,dt = \int_0^{\infty} g_a(x,t)\,dt/g_a(x,\infty). \tag{5.5.45}$$

Simply integrating (5.5.44) with respect to t, we get

$$A(x)\partial_x[\pi_a(x)T(a,x)] + \tfrac{1}{2}B(x)\partial_x^2[\pi_a(x)T(a,x)] = -\pi_a(x), \tag{5.5.46}$$

where we define

$$\pi_a(x) = (\text{probability of exit through } a) = g_a(x,0). \tag{5.5.47}$$

The boundary conditions on (5.5.46) are quite straightforward since they follow from those for the backward Fokker-Planck equation, namely,

$$\pi_a(a)T(a,a) = \pi_a(b)T(a,b) = 0. \tag{5.5.48}$$

In the first of these clearly $T(a,a)$ is zero (the time to reach a from a is zero) and in the second, $\pi_a(b)$ is zero (the probability of exiting through a, starting from b, is zero).

By letting $t \to 0$ in (5.5.44), we see that $J(a,0|x,0)$ must vanish if $a \neq x$, since. $p(a,0\,|\,x,0) = \delta(x-a)$. Hence, the right-hand side tends to zero and we get

$$A(x)\partial_x \pi_a(x) + \tfrac{1}{2}B(x)\partial_x^2 \pi_a(x) = 0\,, \tag{5.5.49}$$

the boundary condition this time being

$$\pi_a(a) = 1, \quad \pi_a(b) = 0\,. \tag{5.5.50}$$

The solution of (5.5.49) subject to this boundary condition and the condition

$$\pi_a(x) + \pi_b(x) = 1\,, \tag{5.5.51}$$

is

$$\pi_a(x) = \left[\int_x^b dy\,\psi(y)\right] \Big/ \int_a^b dy\,\psi(y), \tag{5.5.52}$$

$$\pi_b(x) = \left[\int_a^x dy\,\psi(y)\right] \Big/ \int_a^b dy\,\psi(y)\,. \tag{5.5.53}$$

with $\psi(x)$ as defined in (5.5.20).

These formulae find application in the problem of relaxation of a distribution initially concentrated at an unstable stationary point (Sect. 14.1.4).

Example—Diffusive Traversal Time of a One-Dimensional medium: A particle diffuses in a one-dimension according to the diffusion equation $\partial_t p = \frac{1}{2}D\partial_x^2 p$. What is the mean time for the particle to diffuse from b to a under the condition that it does not leave the interval (a,b) before reaching a? [5.6]

In the case that the particle starts at x within (a,b), we find from (5.5.52) and (5.5.46)

$$\pi_a(x) = \frac{b-x}{b-a}, \tag{5.5.54}$$

$$\tfrac{1}{2}D\partial_x^2[\pi_a(x)T_a(x)] = -\pi_a(x)\,. \tag{5.5.55}$$

Using the boundary conditions (5.5.48) the second equation is easily integrated to give

$$\pi_a(x)T_a(x) = \frac{(x-b)(x-a)(x+a-2b)}{3D(b-a)}, \tag{5.5.56}$$

and hence

$$T_a(x) = \frac{(x-a)(2b-x-a)}{3D}. \tag{5.5.57}$$

In the limiting case $x \to b$, the probability of exit through a as given by (5.5.54), is zero. Nevertheless, in the limit that x is approaches b, the mean time to make the exit given that the exit is at a is quite well defined and is

$$T_a(b) = \frac{(b-a)^2}{3D}. \tag{5.5.58}$$

This is also clearly the time to exit at a without ever leaving the interval (a,b) before exiting at a.

Semi-infinite interval: Notice that if we fix x and let $b \to \infty$, we find

$$\pi_a(x) \to 1\,, \tag{5.5.59}$$

$$T_a(x) \to \infty\,. \tag{5.5.60}$$

The result is that the particle is certain to escape at a, but the average time to escape is infinite. This arises because the particle can spend a great deal of time exploring the infinite half of the interval, giving rise to an escape time distribution which is normalisable, but decays so slowly that all moments diverge.