From this we have

$$\langle \boldsymbol{x}(t) \rangle = \exp\left[-\int_0^t A(t')dt'\right]\langle \boldsymbol{x}(0) \rangle \tag{4.4.84}$$

$$\langle \boldsymbol{x}(t), \boldsymbol{x}^{\mathrm{T}}(t) \rangle = \exp\left[-\int_0^t A(t')dt'\right]\langle \boldsymbol{x}(0), \boldsymbol{x}(0)^{\mathrm{T}} \rangle \exp\left[-\int_0^t A^{\mathrm{T}}(t')dt'\right]$$

$$+ \int_0^t dt' \exp\left[-\int_{t'}^t A(s)ds\right] B(t')B^{\mathrm{T}}(t') \exp\left[-\int_{t'}^t A^{\mathrm{T}}(s)ds\right]. \tag{4.4.85}$$

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 this rather long chapter, 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. The chapter divides into two main subjects—single variable and multivariable processes. There are a large number of exact results for single variable systems, which makes the separate treatment of such systems appropriate. Thus Sect. 5.2 and its subsections treat all aspects of one variable systems, whereas Sect. 5.3 deals with multivariable systems. However, the construction of appropriate boundary conditions is of fundamental importance in both cases, and is carried out in general in Sect. 5.2.1. A corresponding treatment for the boundary conditions on the backward Fokker-Planck equation is given in Sect. 5.2.4. The remaining subsections of Sect. 5.2 are 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.

Section 5.3 and its subsections explore exact results for many variable systems. These results are not as explicit as for the one variable case. An extra feature which is included is the concept of *detailed balance* in multivariable systems, which is almost trivial in one variable systems, but leads to very interesting conclusions in multivariable systems.

The chapter concludes with a treatment of exact results in exit problems for multivariable Fokker-Planck equations.

5.1 Background

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.4.3.4). 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] 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 which this book is addressed.

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.3.4,5, the FPE 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

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

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

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

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

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

$$\partial_t p(\boldsymbol{z},t) = -\sum_i \frac{\partial}{\partial z_i} A_i(\boldsymbol{z},t)p(\boldsymbol{z},t) + \frac{1}{2}\sum_{i,j}\frac{\partial^2}{\partial z_i \partial z_j} B_{ij}(\boldsymbol{z},t)p(\boldsymbol{z},t) \tag{5.2.6}$$

We note that this can also be written

$$\frac{\partial p(\boldsymbol{z},t)}{\partial t} + \sum_i \frac{\partial}{\partial z_i} J_i(\boldsymbol{z},t) = 0 \tag{5.2.7}$$

where we define the *probability current*

$$J_i(\boldsymbol{z},t) = A_i(\boldsymbol{z},t)\,p(\boldsymbol{z},t) - \frac{1}{2}\sum_j \frac{\partial}{\partial z_j} B_{ij}(\boldsymbol{z},t)p(\boldsymbol{z},t) \tag{5.2.8}$$

Equation (5.2.7) 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 $\boldsymbol{S}$ and define

$$P(R,t) = \int_R d\boldsymbol{z}\, p(\boldsymbol{z},t)$$

then (5.2.7) is equivalent to

$$\frac{\partial P(R,t)}{\partial t} = -\int_S dS\, \boldsymbol{n}\cdot\boldsymbol{J}(\boldsymbol{z},t) \tag{5.2.9}$$

where $\boldsymbol{n}$ is the outward pointing normal to $\boldsymbol{S}$. Thus (5.2.9) indicates that the total loss of probability is given by the surface integral of $\boldsymbol{J}$ over the boundary of R. We can show as well that the current $\boldsymbol{J}$ does have the somewhat stronger property, that a surface integral over any surface $\boldsymbol{S}$ gives the net flow of probability across that surface.

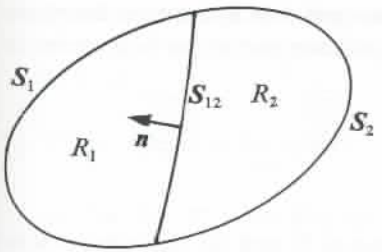

Fig. 5.1. Regions used to demonstrate that the probability current is the flow of probability

For consider two adjacent regions R_1 and R_2, separated by a surface $\boldsymbol{S}_{12}$. Let $\boldsymbol{S}_1$ and $\boldsymbol{S}_2$ be the surfaces which, together with $\boldsymbol{S}_{12}$, 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 $t + \Delta t$,

$$= \int_{R_1} dx \int_{R_2} dy\, p(x, t + \Delta t; y, t).$$

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.

$$\lim_{\Delta t \to 0} \frac{1}{\Delta t} \int_{R_1} dx \int_{R_2} dy\, [p(x, t + \Delta t; y, t) - p(y, t + \Delta t; x, t)]. \tag{5.2.10}$$

Note that

$$\int_{R_1} dx \int_{R_2} dy\, p(x, t; y, t) = 0$$

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

$$(5.2.10) = \int_{R_1} dx \int_{R_2} dy\, [\partial_{t'} p(x, t'; y, t) - \partial_{t'} p(y, t'; x, t)]_{t'=t}$$

and using the Fokker-Planck equation in the form (5.2.7)

$$= -\int_{R_1} dx \sum_i \frac{\partial}{\partial x_i} J_i(x, t; R_2, t) + \int_{R_2} dy \sum_i \frac{\partial}{\partial y_i} J_i(y, t; R_1, t) \tag{5.2.11}$$

where $J_i(x, t; R_2, t)$ is formed from

$$p(x, t; R_2, t) = \int_{R_2} dy\, p(x, t; y, t)$$

in the same way as $J(z, t)$ is formed from $p(z, t)$ in (5.2.8) and $J_i(y, t; R_1, t)$ is defined similarly. We now convert the integrals to surface integrals. The integral over S_2 vanishes, since it will involve $p(x, t; R_2, t)$, with 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

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

and we finally conclude, since 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

$$\equiv \lim_{\Delta t \to 0} \frac{1}{\Delta t} \int_{R_1} dx \int_{R_2} dy\, [p(x, t + \Delta t; y, t) - p(y, t + \Delta t; x, t)] = \int_{S_{12}} dS\, n \cdot J(x, t) \tag{5.2.12}$$

where n points from R_2 to R_1

We can now consider the various boundary conditions 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

$$n \cdot J(z, t) = 0 \quad \text{for } z \in S, \quad n = \text{normal to } S \tag{5.2.13}$$

where $J(z, t)$ is given by (5.2.8).

Since the particle cannot cross S, it must be reflected there, and hence the name *reflecting barrjer* for this condition.

b) Absorbing Barrier

Here, one assumes that the moment the particle reaches S, it is removed from the system, thus the barrier absorbs. Consequently, the probability of being on the boundary is zero, i.e.

$$p(z, t) = 0 \qquad \text{for } z \in S \tag{5.2.14}$$

c) Boundary Conditions at a Discontinuity

It is possible for both the A_i and B_{ij} coefficients to be discontinuous at a surface S, but for there to be free motion across S. Consequently, the probability and the normal component of the current must both be continuous across S,

$$n \cdot J(z)|_{S_+} = n \cdot J(z)|_{S_-} \tag{5.2.15}$$

$$p(z)|_{S_+} = p(z)|_{S_-} \tag{5.2.16}$$

where S_+, S_-, as subscripts, mean the limits of the quantities from the left and right hand sides of the surface.

The definition (5.2.8) of the current, indicates that the derivatives of $p(z)$ are not necessarily continuous at S.

d) 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.,

$$\text{I: } \lim_{x \to b-} p(x, t) = \lim_{x \to a+} p(x, t) \tag{5.2.17}$$

$$\text{II: } \lim_{x \to b-} J(x, t) = \lim_{x \to a+} J(x, t). \tag{5.2.18}$$

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

$$\begin{aligned} A(b, t) &= A(a, t) \\ B(b, t) &= B(a, t) \end{aligned} \tag{5.2.19}$$

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.

e) 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. 4.3.1) and $B(x, t)$ is differentiable at $x = a$ then

$$\partial_x B(a, t) = 0 . \tag{5.2.20}$$

The SDE then has solutions, and we may write

$$dx(t) = A(x, t)\, dt + \sqrt{B(x, t)}\, dW(t) \tag{5.2.21}$$

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

$$A(a, t) < 0 \tag{5.2.22}$$

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

$$A(a, t) > 0 . \tag{5.2.23}$$

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

$$A(a, t) = 0 . \tag{5.2.24}$$

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.

Feller [5.4] has shown 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

$$f(x) = \exp\left[-2\int_{x_0}^{x} ds\, A(s)/B(s)\right] \tag{5.2.25}$$

$$g(x) = 2/[B(x) f(x)] \tag{5.2.26}$$

$$h_1(x) = f(x) \int_{x_0}^{x} g(s)\, ds \tag{5.2.27}$$

$$h_2(x) = g(x) \int_{x_0}^{x} f(s)\, ds . \tag{5.2.28}$$

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

$$\mathcal{L}(x_1, x_2) \tag{5.2.29}$$

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 $f(x) \in \mathcal{L}(a, x_0)$, and $g(x) \in \mathcal{L}(a, x_0)$

II: Exit: if $g(x) \notin \mathcal{L}(a, x_0)$, and $h_1(x) \in \mathcal{L}(a, x_0)$

III: Entrance: if $g(x) \in \mathcal{L}(a, x_0)$, and $h_2(x) \in \mathcal{L}(a, x_0)$

IV: Natural : all other cases.

It can be seen from the results of Sect. 5.2.2 that for an exit boundary there is no normalisable stationary solution of the FPE, and that the mean time to reach the boundary, (5.2.161), 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 [5.5] for a more complete description.

f) 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

$$\lim_{x \to \infty} p(x, t) = 0 . \tag{5.2.30}$$

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

$$\lim_{x \to \infty} \partial_x p(x, t) = 0 \tag{5.2.31}$$

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:

i) $J(\pm\infty, t) = 0$ (5.2.32)

ii) $J(+\infty, t) = J(-\infty, t)$. (5.2.33)

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

5.2.2 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

$$\frac{d}{dx}[A(x)p_s(x)] - \frac{1}{2}\frac{d^2}{dx^2}[B(x)p_s(x)] = 0 \tag{5.2.34}$$

which can also be written simply in terms of the current (as defined in Sect.5.2.1)

$$\frac{dJ(x)}{dx} = 0 \tag{5.2.35}$$

which clearly has the solution

$$J(x) = \text{constant}. \tag{5.2.36}$$

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

$$J(a) = J(x) = J(b) \equiv J \tag{5.2.37}$$

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

If the boundaries are not reflecting, (5.2.37) requires them to be periodic. We then use the boundary conditions given by (5.2.17,18).

a) Zero Current—Potential Solution

Setting $J = 0$, we rewrite (5.2.37) as

$$A(x)p_s(x) = \frac{1}{2}\frac{d}{dx}[B(x)p_s(x)] = 0 \tag{5.2.38}$$

for which the solution is

$$p_s(x) = \frac{\mathcal{N}}{B(x)}\exp[2\int_a^x dx' A(x')/B(x')], \tag{5.2.39}$$

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

$$\int_a^b dx\, p_s(x) = 1. \tag{5.2.40}$$

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.5.3.3).

b) Periodic Boundary Condition

Here we have nonzero current J and we rewrite (5.2.36) as

$$A(x)p_s(x) - \frac{1}{2}\frac{d}{dx}[B(x)p_s(x)] = J. \tag{5.2.41}$$

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

$$p_s(a) = p_s(b) \tag{5.2.42}$$

$$J(a) = J(b). \tag{5.2.43}$$

For convenience, define

$$\psi(x) = \exp[2\int_a^x dx' A(x')/B(x')]. \tag{5.2.44}$$

Then we can easily integrate (5.2.41) to get

$$p_s(x)B(x)/\psi(x) = p_s(a)B(a)/\psi(a) - 2J\int_a^x dx'/\psi(x'). \tag{5.2.45}$$

By imposing the boundary condition (5.2.42) we find that

$$J = [B(b)/\psi(b) - B(a)/\psi(a)]p_s(a)/\left[\int_a^b dx'/\psi(x')\right] \tag{5.2.46}$$

so that

$$p_s(x) = p_s(a)\left[\frac{\int_a^x \frac{dx'}{\psi(x')}\frac{B(b)}{\psi(b)} + \int_x^b \frac{dx'}{\psi(x')}\frac{B(a)}{\psi(a)}}{\frac{B(x)}{\psi(x)}\int_a^b \frac{dx'}{\psi(x')}}\right]. \tag{5.2.47}$$

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.

5.2.3 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 SDE (Sect.6.4)

$$dx = -g\,dt + \sqrt{D}\,dW(t) \tag{5.2.48}$$

for which the Fokker-Planck equation is

$$\frac{\partial p}{\partial t} = \frac{\partial}{\partial x}(gp) + \frac{1}{2}D\frac{\partial^2 p}{\partial x^2}. \tag{5.2.49}$$

On the interval (a, b) with reflecting boundary conditions, the stationary solution is given by (5.2.39), i.e.

$$p_s(x) = \mathcal{N} \exp\left[-2gx/D\right], \tag{5.2.50}$$

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 (5.2.47) yields

$$p_s(x) = p_s(a); \tag{5.2.51}$$

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

$$\frac{\partial p}{\partial t} = \frac{\partial}{\partial x}(kxp) + \frac{1}{2}D\frac{\partial^2 p}{\partial x^2}, \tag{5.2.52}$$

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

$$p_s(x) = \mathcal{N} \exp\left(-kx^2/D\right). \tag{5.2.53}$$

Provided $k > 0$, this is normalisable on $(-\infty, \infty)$. If $k < 0$, one can only make sense of it on a finite interval.

Suppose

$$a = -b < 0\,. \tag{5.2.54}$$

Then in this case,

$$\psi(x) = \exp\left[-\frac{k}{D}(x^2 - a^2)\right] \tag{5.2.55}$$

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

$$\psi(a) = \psi(-a), \tag{5.2.56}$$

we find that

$$\begin{aligned} p_s(x) &= p_s(a)\psi(x)/\psi(a) \\ &= p_s(a)\exp\left[-\frac{k}{D}(x^2 - a^2)\right] \end{aligned}$$

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. 7), approximate treatments are often given by means of a FPE. The reaction

$$X + A \rightleftharpoons 2X \tag{5.2.57}$$

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 FPE is derived in Sect.7.6.1 and is

$$\partial_t p(x, t) = -\partial_x[(ax - x^2)p(x, t)] + \tfrac{1}{2}\partial_x^2[(ax + x^2)p(x, t)]\,. \tag{5.2.58}$$

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

$$p_s(x) = e^{-2x}(a + x)^{4a-1}x^{-1} \tag{5.2.59}$$

which is not normalisable if $\alpha = 0$. The pole at $x = 0$ is a result of the absorption there. In fact, comparing with (5.2.28), we see that

$$\begin{aligned} B(0, t) &\equiv (ax + x^2)_{x=0} = 0 \\ A(0, t) &\equiv (ax - x^2)_{x=0} = 0 \\ \partial_x B(0, t) &\equiv (a + 2x)_{x=0} > 0 \end{aligned} \tag{5.2.60}$$

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 (5.2.59) is, in practice, a good representation of the distribution except near $x = 0$.

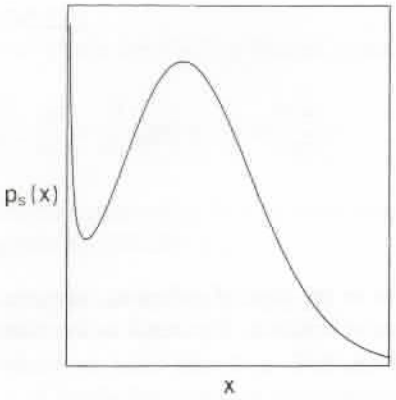

Fig. 5.2. Non-normalisable "stationary" $p_s(x)$ for the reaction $X + A \rightleftharpoons 2X$

5.2.4 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',

$$0 = \frac{\partial}{\partial s} p(\boldsymbol{x}, t|\boldsymbol{x}', t') = \frac{\partial}{\partial s} \int d\boldsymbol{y} p(\boldsymbol{x}, t|\boldsymbol{y}, s) p(\boldsymbol{y}, s|\boldsymbol{x}', t') , \tag{5.2.61}$$

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

$$\begin{aligned} p(\boldsymbol{y}, s) &= p(\boldsymbol{y}, s|\boldsymbol{x}', t') \\ \bar{p}(\boldsymbol{y}, s) &= p(\boldsymbol{x}, t|\boldsymbol{y}, s) . \end{aligned} \tag{5.2.62}$$

Then,

$$\begin{aligned} 0 = &\int_R d\boldsymbol{y} \left[-\sum_i \frac{\partial}{\partial y_i}(A_i p) + \sum_{i,j} \frac{\partial^2}{\partial y_i \partial y_j}(B_{ij} p) \right] \bar{p} \\ &+ \int_R d\boldsymbol{y} \left[-\sum_i A_i \frac{\partial \bar{p}}{\partial y_i} - \sum_{i,j} B_{ij} \frac{\partial^2 \bar{p}}{\partial y_i \partial y_j} \right] p \end{aligned} \tag{5.2.63}$$

and after some manipulation

$$= \int_R d\boldsymbol{y} \sum_i \frac{\partial}{\partial y_i} \left[-A_i p \bar{p} + \frac{1}{2} \sum_j \left[\bar{p} \frac{\partial}{\partial y_j}(B_{ij} p) - p B_{ij} \frac{\partial \bar{p}}{\partial y_j} \right] \right] \tag{5.2.64}$$

$$= \int_S \sum_i dS_i \left\{ \bar{p} \left[-A_i p + \frac{1}{2} \sum_j \frac{\partial}{\partial y_i}(B_{ij} p) \right] \right\} - \frac{1}{2} \int_S \sum_i dS_i p \left(\sum_j B_{ij} \frac{\partial \bar{p}}{\partial y_j} \right) . \tag{5.2.65}$$

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 (5.2.65) since on substituting $p = 0$ in that equation, we get

$$0 = \int_S \bar{p} \sum_{i,j} dS_i B_{ij} \frac{\partial p}{\partial y_j} . \tag{5.2.66}$$

However, if the boundary is absorbing, clearly

$$p(\boldsymbol{x}, t|\boldsymbol{y}, s) = 0, \qquad \text{for } \boldsymbol{y} \in \text{boundary} \tag{5.2.67}$$

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 (5.2.65). The final factor vanishes for arbitrary p only if

$$\sum_{i,j} n_i B_{ij}(\boldsymbol{y}) \frac{\partial}{\partial y_j} [p(\boldsymbol{x}, t|\boldsymbol{y}, s)] = 0 . \tag{5.2.68}$$

In one dimension this reduces to

$$\frac{\partial}{\partial y} p(\boldsymbol{x}, t|\boldsymbol{y}, s) = 0 \tag{5.2.69}$$

unless B vanishes.

c) Other Boundaries

We shall not consider these in this section. For further details see [5.4].

5.2.5 Eigenfunction Methods (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.

a) Eigenfunctions for Reflecting Boundaries

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

$$\partial_t p(x,t) = -\partial_x[A(x)p(x,t)] + \tfrac{1}{2}\,\partial_x^2[B(x)p(x,t)]\,. \tag{5.2.70}$$

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

$$p(x,t) = p_s(x)q(x,t) \tag{5.2.71}$$

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

$$\partial_t q(x,t) = A(x)\partial_x q(x,t) + \tfrac{1}{2}\,B(x)\partial_x^2 q(x,t)\,. \tag{5.2.72}$$

We now wish to consider solutions of the form

$$p(x,t) = P_\lambda(x)\mathrm{e}^{-\lambda t} \tag{5.2.73}$$

$$q(x,t) = Q_\lambda(x)\mathrm{e}^{-\lambda t} \tag{5.2.74}$$

which obey the eigenfunction equations

$$-\partial_x[A(x)P_\lambda(x)] + \tfrac{1}{2}\,\partial_x^2[B(x)P_\lambda(x)] = -\lambda P_\lambda(x) \tag{5.2.75}$$

$$A(x)\partial_x Q_{\lambda'}(x) + \tfrac{1}{2}\,B(x)\partial_x^2 Q_{\lambda'}(x) = -\lambda' Q_{\lambda'}(x)\,. \tag{5.2.76}$$

Then we can straightforwardly show by partial integration that

$$(\lambda' - \lambda)\int_a^b dx P_\lambda(x)Q_{\lambda'}(x) = [Q_{\lambda'}(x)\{-A(x)P_\lambda(x) + \tfrac{1}{2}\,\partial_x[B(x)P_\lambda(x)]\} - \tfrac{1}{2}\,B(x)P_\lambda(x)\partial_x Q_{\lambda'}(x)]_a^b, \tag{5.2.77}$$

and using the reflecting boundary condition on the coefficient of $Q_{\lambda'}(x)$, we see that it vanishes. Further, using the definition of $q(x,t)$ in terms of the stationary solution (5.2.71), it is simple to show that

$$\tfrac{1}{2}\,B(x)\partial_x Q_{\lambda'}(x) = -A(x)P_{\lambda'}(x) + \tfrac{1}{2}\,\partial_x[B(x)P_{\lambda'}(x)] \tag{5.2.78}$$

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

$$\int_a^b dx\; P_\lambda(x)Q_{\lambda'}(x) = \delta_{\lambda\lambda'} \tag{5.2.79}$$

or, there are two alternative orthogonality systems,

$$\int_a^b dx\; p_s(x)Q_\lambda(x)Q_{\lambda'}(x) = \delta_{\lambda\lambda'} \tag{5.2.80}$$

$$\int_a^b dx[p_s(x)]^{-1}P_\lambda(x)P_{\lambda'}(x) = \delta_{\lambda\lambda'}\,. \tag{5.2.81}$$

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

$$P_0(x) = p_s(x) \tag{5.2.82}$$

$$Q_0(x) = 1\,. \tag{5.2.83}$$

Using this orthogonality we can write any solution in terms of eigenfunctions. For if

$$p(x,t) = \sum_\lambda A_\lambda P_\lambda(x)\mathrm{e}^{-\lambda t}\,, \tag{5.2.84}$$

then

$$\int_a^b dx\; Q_\lambda(x)p(x,0) = A_\lambda\,. \tag{5.2.85}$$

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

$$p(x,0|x_0,0) = \delta(x - x_0) \tag{5.2.86}$$

so that

$$A_\lambda = \int_a^b dx\; Q_\lambda(x)\delta(x - x_0) = Q_\lambda(x_0) \tag{5.2.87}$$

and hence,

$$p(x,t|x_0,0) = \sum_\lambda P_\lambda(x)Q_\lambda(x_0)\mathrm{e}^{-\lambda t}\,. \tag{5.2.88}$$

We can write the autocorrelation function quite elegantly as

$$\langle x(t)x(0)\rangle = \int dx \int dx_0\; xx_0 p(x,t|x_0,0)p_s(x) \tag{5.2.89}$$

$$= \sum_\lambda \left[\int dx\; xP_\lambda(x)\right]^2 \mathrm{e}^{-\lambda t}\,, \tag{5.2.90}$$

where we have used the definition of $Q_\lambda(x)$ by (5.2.74).

b) Eigenfunctions for Absorbing Boundaries

This is very similar. 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

$$P_\lambda(a) = Q_\lambda(a) = P_\lambda(b) = Q_\lambda(b) = 0 \tag{5.2.91}$$

and the orthogonality proof still follows through. Eigenfunctions are then computed using this condition and the eigenfunction equations (5.2.75, 76) 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 $t \to \infty$.

5.2.6 Examples

a) A Wiener Process with Absorbing Boundaries

The Fokker-Planck equation

$$\partial_t p = \tfrac{1}{2}\partial_x^2 p \tag{5.2.92}$$

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

$$p(0, t) = p(1, t) = 0 \tag{5.2.93}$$

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

$$p(x, t) = \sum_{n=1}^{\infty} b_n(t) \sin(n\pi x) \tag{5.2.94}$$

which automatically satisfies (5.2.93). The initial condition is chosen so that

$$p(x, 0) = \delta(x - x_0) \tag{5.2.95}$$

for which the Fourier coefficients are

$$b_n(0) = 2\int_0^1 dx\, \delta(x - x_0) \sin(n\pi x) = 2 \sin(n\pi x_0)\,. \tag{5.2.96}$$

Substituting the Fourier expansion (5.2.94) into (5.2.92) gives

$$\dot{b}_n(t) = -\lambda_n b_n(t) \tag{5.2.97}$$

with

$$\lambda_n = n^2\pi^2/2 \tag{5.2.98}$$

and the solution

$$b_n(t) = b_n(0)\exp(-\lambda_n t)\,. \tag{5.2.99}$$

So we have the solution [which by the initial condition (5.2.95) is for the conditional probability $p(x, t|x_0, 0)$]

$$p(x, t|x_0, 0) = 2\sum_{n=1}^{\infty} \exp(-\lambda_n t) \sin(n\pi x_0) \sin(n\pi x)\,. \tag{5.2.100}$$

b) Wiener Process with Reflecting Boundaries

Here the boundary condition reduces to [on the interval (0, 1)]

$$\partial_x p(0, t) = \partial_x p(1, t) = 0 \tag{5.2.101}$$

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

$$p(x, t) = \frac{1}{2} a_0 + \sum_{n=1}^{\infty} a_n(t) \cos(n\pi x) \tag{5.2.102}$$

with the same initial condition

$$p(x, 0) = \delta(x - x_0) \tag{5.2.103}$$

so that

$$a_n(0) = 2\int_0^1 dx \cos(n\pi x)\delta(x - x_0) = 2\cos(n\pi x_0)\,. \tag{5.2.104}$$

In the same way as before, we find

$$a_n(t) = a_n(0) \exp(-\lambda_n t) \tag{5.2.105}$$

with

$$\lambda_n = n^2\pi^2/2 \tag{5.2.106}$$

so that

$$p(x, t|x_0, 0) = 1 + 2\sum_{n=1}^{\infty} \cos(n\pi x_0) \cos(n\pi x) \exp(-\lambda_n t)\,. \tag{5.2.107}$$

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

$$p_s(x) = \lim_{t\to\infty} p(x, t|x_0, 0) = 1\,. \tag{5.2.108}$$

We can compute the stationary autocorrelation function by

$$\langle x(t)x(0)\rangle_s = \int_0^1\int_0^1 dx\, dx_0\, x x_0 p(x, t|x_0, 0) p_s(x) \tag{5.2.109}$$

and carrying out the integrals explicitly,

$$\langle x(t)x(0)\rangle_s = \frac{1}{4} + \frac{8}{\pi^4}\sum_{n=0}^{\infty} \exp(-\lambda_{2n+1} t)\,(2n + 1)^{-4}\,. \tag{5.2.110}$$

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

$$\langle x(t)x(0)\rangle_s \to \tfrac{1}{4} = [\langle x\rangle_s]^2 \tag{5.2.111}$$

and as $t \to 0$,

$$\langle x(t)x(0)\rangle_s \to \frac{1}{4} + \frac{8}{\pi^4}\sum_{n=0}^{\infty}(2n+1)^{-4} = \frac{1}{3} = \langle x_s^2\rangle \tag{5.2.113}$$

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

$$\sum_{n=0}^{\infty}(2n+1)^{-4} = \frac{\pi^4}{96}. \tag{5.2.114}$$

c) Ornstein-Uhlenbeck Process

As in Sect.3.8.4, the Fokker-Planck equation is

$$\partial_t p(x,t) = \partial_x[kxp(x,t)] + \tfrac{1}{2}D\partial_x^2 p(x,t)\,. \tag{5.2.115}$$

The eigenfunction equation for Q_λ is

$$d_x^2 Q_\lambda - \frac{2kx}{d}d_x Q_\lambda + \frac{2\lambda}{D}Q_\lambda = 0 \tag{5.2.116}$$

and this becomes the differential equation for *Hermite polynomials* [5.6] on making the replacement

$$\begin{aligned} &y = x\sqrt{k/D} \\ &d_y^2 Q_\lambda - 2yd_y Q_\lambda + (2\lambda/k)Q_\lambda = 0\,. \end{aligned} \tag{5.2.117}$$

We can write

$$Q_\lambda = (2^n n!)^{-1/2}\mathrm{H}_n(x\sqrt{k/D})\,, \tag{5.2.118}$$

where

$$\lambda = nk\,, \tag{5.2.119}$$

and these solutions are normalised as in (5.2.79–81).

The stationary solution is, as previously found,

$$p_s(x) = (k/\pi D)^{1/2}\exp(-kx^2/D) \tag{5.2.120}$$

and a general solution can be written as

$$p(x,t) = \sum_n \sqrt{[k/(2^n n!\pi D)]}\exp(-kx^2/D)\mathrm{H}_n(x\sqrt{k/D})\mathrm{e}^{-nkt}A_n \tag{5.2.121}$$

with

$$A_n = \int_{-\infty}^{\infty} dx\; p(x,0)\mathrm{H}_n(x\sqrt{k/D})(2^n n!)^{-1/2}\,. \tag{5.2.122}$$

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

$$\lambda_n = nk. \tag{5.2.123}$$

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 (5.2.90). We use the result [5.6] that

$$\mathrm{H}_1(y) = 2y \tag{5.2.124}$$

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

$$\begin{aligned} \int x\,P_{\lambda_1}(x)dx &= \int_{-\infty}^{\infty}\sqrt{k/(2\pi D)}\exp(-kx^2/D)(2x\sqrt{k/D})x \\ &= \sqrt{D/2k} \end{aligned} \tag{5.2.125}$$

so that

$$\langle x(t)x(0)\rangle_s = \frac{D}{2k}\mathrm{e}^{-kt}\,, \tag{5.2.126}$$

as found previously in Sects.3.8.4, 4.4.4.

d) Rayleigh Process

We take the model of amplitude fluctuations developed in Sect.4.4.5. The Fokker-Planck equation is

$$\partial_t p(x,t) = \partial_x[(\gamma x - \mu/x)p(x,t)] + \mu\partial_x^2 p(x,t)\,, \tag{5.2.127}$$

where

$$\mu = \varepsilon^2/2\,. \tag{5.2.128}$$

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

$$p_s(x) = (\gamma x/\mu)\exp(-\gamma x^2/2\mu)\,. \tag{5.2.129}$$

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

$$d_x^2 Q_\lambda + (1/x - \gamma x/\mu)d_x Q_\lambda + (\lambda/\mu)Q_\lambda = 0\,. \tag{5.2.130}$$

By setting

$$z = x^2\gamma/2\mu\,, \tag{5.2.131}$$

we obtain

$$z d_z^2 Q_\lambda + (1 - z) d_z Q_\lambda + (\lambda/2\gamma) Q_\lambda = 0 . \tag{5.2.132}$$

This is the differential equation for the *Laguerre polynomials* [5.6] provided

$$\lambda = 2n\gamma . \tag{5.2.133}$$

We can write

$$Q_\lambda(x) = \mathrm{L}_n(\gamma x^2/2\mu) \tag{5.2.134}$$

which is normalised. Hence, the conditional probability is

$$p(x, t \mid x_0, 0) = \sum_{n=0}^{\infty} \frac{\gamma x}{\mu} \exp\left(-\frac{\gamma x^2}{2\mu}\right) \mathrm{L}_n\left(\frac{\gamma x_0^2}{2\mu}\right) \mathrm{L}_n\left(\frac{\gamma x^2}{2\mu}\right) \mathrm{e}^{-2n\gamma t} . \tag{5.2.135}$$

We can compute the autocorrelation function by the method of (5.2.90):

$$\langle x(t) x(0) \rangle = \sum_{n=0}^{\infty} \left[\int_0^{\infty} x \, dx \, \frac{\gamma x}{\mu} \exp\left(\frac{-\gamma x^2}{2\mu}\right) \mathrm{L}_n\left(\frac{\gamma x^2}{2\mu}\right) \right]^2 \exp(-2n\gamma t) \tag{5.2.136}$$

and using

$$\int_0^{\infty} dz \, z^\alpha \mathrm{e}^{-z} \mathrm{L}_n(z) = (-1)^n \Gamma(\alpha + 1) \binom{\alpha}{n} , \tag{5.2.137}$$

we find for the autocorrelation function

$$\langle x(t) x(0) \rangle = \frac{2\mu}{\gamma} \sum_{n=0}^{\infty} \frac{\pi}{4} \left(\frac{1}{2}\right)^2 \exp(-2n\gamma t). \tag{5.2.138}$$

5.2.7 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.

a) 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:

$$a \leqslant x \leqslant b \tag{5.2.139}$$

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.

Under these conditions, the probability that at time t the particle is still in (a, b) is

$$\int_a^b dx' p(x', t \mid x, 0) \equiv G(x, t) . \tag{5.2.140}$$

Let the time that the particle leaves (a, b) be T. Then we can rewrite (5.2.140) as

$$\mathrm{Prob}(T \geqslant t) = \int_a^b dx' p(x', t \mid x, 0) \tag{5.2.141}$$

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

$$p(x', t \mid x, 0) = p(x', 0 \mid x, -t) \tag{5.2.142}$$

and the backward Fokker-Planck equation can be written

$$\partial_t p(x', t \mid x, 0) = A(x) \partial_x p(x', t \mid x, 0) + \tfrac{1}{2} B(x) \partial_x^2 p(x', t \mid x, 0) \tag{5.2.143}$$

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

$$\partial_t G(x, t) = A(x) \partial_x G(x, t) + \tfrac{1}{2} B(x) \partial_x^2 G(x, t) . \tag{5.2.144}$$

The boundary conditions are clearly that

$$p(x', 0 \mid x, 0) = \delta(x - x')$$

and hence,

$$\begin{aligned} G(x, 0) &= 1 \qquad a \leqslant x \leqslant b \\ &= 0 \qquad \text{elsewhere} \end{aligned} \tag{5.2.145}$$

and if $x = a$ or b, the particle is absorbed immediately, so

$$\begin{aligned} &\mathrm{Prob}(T \geqslant t) = 0 \qquad \text{when } x = a \text{ or } b , \qquad \text{i.e.,} \\ &G(a, t) = G(b, t) = 0. \end{aligned} \tag{5.2.146}$$

Since $G(x, t)$ is the probability that $T \geqslant t$, the mean of any function of T is

$$\langle f(T) \rangle = -\int_0^{\infty} f(t) dG(x, t) . \tag{5.2.147}$$

Thus, the *mean first passage time*

$$T(x) = \langle T \rangle \tag{5.2.148}$$

is given by

$$T(x) = -\int_0^{\infty} t \, \partial_t G(x, t) dt \tag{5.2.149}$$

$$= \int_0^\infty G(x, t)dt \tag{5.2.150}$$

after integrating by parts.

Similarly, defining

$$T_n(x) = \langle T^n \rangle , \tag{5.2.151}$$

we find

$$T_n(x) = \int_0^\infty t^{n-1} G(x, t)dt . \tag{5.2.152}$$

We can derive a simple ordinary differential equation for $T(x)$ by using (5.2.150) and integrating (5.2.144) over $(0, \infty)$. Noting that

$$\int_0^\infty \partial_t G(x, t)dt = G(x, \infty) - G(x, 0) = -1 , \tag{5.2.153}$$

we derive

$$A(x)\partial_x T(x) + \tfrac{1}{2} B(x)\partial_x^2 T(x) = -1 \tag{5.2.154}$$

with the boundary condition

$$T(a) = T(b) = 0 . \tag{5.2.155}$$

Similarly, we see that

$$-nT_{n-1}(x) = A(x)\partial_x T_n(x) + \tfrac{1}{2} B(x)\partial_x^2 T_n(x) \tag{5.2.156}$$

which means that all the moments of the first passage time can be found by repeated integration.

Solutions of the Equations. Equation (5.2.154) can be solved directly by integration. The solution, after some manipulation, can be written in terms of

$$\boxed{\psi(x) = \exp\left\{\int_a^x dx'[2A(x')/B(x')]\right\} .} \tag{5.2.157}$$

We find

$$T(x) = \frac{2\left[\left(\int_a^x \frac{dy}{\psi(y)}\right)\int_x^b \frac{dy'}{\psi(y')}\int_a^{y'} \frac{dz\psi(z)}{B(z)} - \left(\int_x^b \frac{dy}{\psi(y)}\right)\int_a^x \frac{dy'}{\psi(y')}\int_a^{y'} \frac{dz\psi(z)}{B(z)}\right]}{\int_a^b \frac{dy}{\psi(y)}} . \tag{5.2.158}$$

b) 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

$$\partial_x G(a, t) = 0 \tag{5.2.159a}$$

$$G(b, t) = 0 \tag{5.2.159b}$$

which follow from the conditions on the backward Fokker-Planck equation derived in Sect.5.2.4. We solve (5.2.154) with the corresponding boundary condition and obtain

$$\boxed{T(x) = 2\int_x^b \frac{dy}{\psi(y)}\int_a^y \frac{\psi(z)}{B(z)}dz \qquad \begin{array}{l} a \text{ reflecting} \\ b \text{ absorbing} \\ a < b \end{array} .} \tag{5.2.160}$$

Similarly, one finds

$$\boxed{T(x) = 2\int_a^x \frac{dy}{\psi(y)}\int_y^b \frac{\psi(z)}{B(z)}dz \qquad \begin{array}{l} b \text{ reflecting} \\ a \text{ absorbing} \\ a < b \end{array} .} \tag{5.2.161}$$

c) Application—Escape Over a Potential Barrier

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

$$\partial_t p(x, t) = \partial_x[U'(x)p(x, t)] + D\partial_x^2 p(x, t) . \tag{5.2.162}$$

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

$$p_s(x) = \mathcal{N} \exp[-U(x)/D] \tag{5.2.163}$$

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 (5.2.160) with the substitutions

$$\begin{aligned} b &\to x_0 \\ a &\to -\infty \\ x &\to a \end{aligned} \tag{5.2.164}$$

so that

$$T(a \to x_0) = \frac{1}{D}\int_a^{x_0} dy \exp[U(y)/D]\int_{-\infty}^y \exp[-U(z)/D]dz . \tag{5.2.165}$$

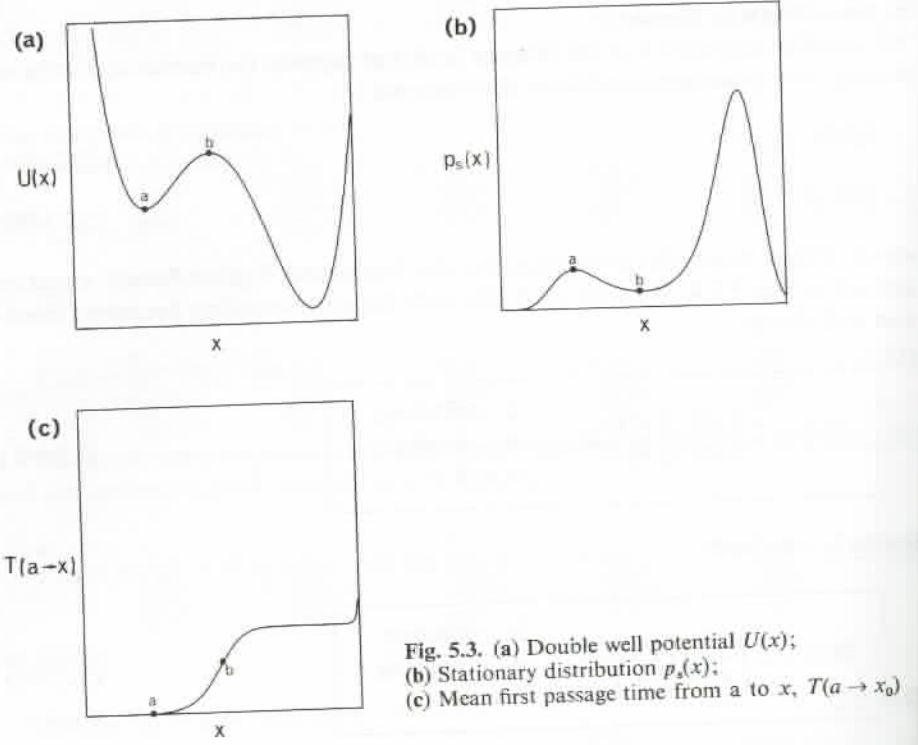

Fig. 5.3. (a) Double well potential $U(x)$;
(b) Stationary distribution $p_s(x)$;
(c) Mean first passage time from a to x, $T(a \to x_0)$

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. Hence, we can approximate (5.2.165) by

$$T(a \to x_0) \simeq \left\{\frac{1}{D}\int_{-\infty}^{b} dy \exp[-U(z)/D]\right\}\int_{a}^{x_0} dy \exp[U(y)/D]\,. \tag{5.2.166}$$

Notice that by the definition of $p_s(x)$ in (5.2.163), we can say that

$$\int_{-\infty}^{b} dy \exp[-U(z)/D] = n_a/\mathcal{N} \tag{5.2.167}$$

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

$$U(x) \simeq U(b) - \frac{1}{2}\left(\frac{x-b}{\delta}\right)^2 \tag{5.2.168}$$

and near a

$$U(x) \simeq U(a) + \frac{1}{2}\left(\frac{x-a}{\alpha}\right)^2. \tag{5.2.169}$$

The constant factor in (5.2.166) is evaluated as

$$\int_{-\infty}^{b} dz \exp[-U(z)/D] \sim \int_{-\infty}^{\infty} dz \exp\left[-\frac{U(a)}{D} - \frac{(z-a)^2}{2D\alpha^2}\right] \tag{5.2.170}$$

$$\sim \alpha\sqrt{2\pi D} \exp[-U(a)/D] \tag{5.2.171}$$

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

$$\int_{a}^{x_0} dy \exp U(y)/D \sim \int_{-\infty}^{\infty} dy \exp\left[\frac{U(b)}{D} - \frac{(y-b)^2}{2D\delta^2}\right] \tag{5.2.172}$$

$$= \delta\sqrt{2\pi D} \exp[U(b)/D]\,. \tag{5.2.173}$$

Putting both of these in (5.2.166), we get

$$T(a \to x_0) \simeq 2\alpha\delta\pi \exp\{[U(b) - U(a)]/D\}\,. \tag{5.2.174}$$

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

$$D = kT\,, \tag{5.2.175}$$

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

$$\exp(\Delta E/kT) \tag{5.2.176}$$

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.9.

5.2.8 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

$$g_a(x,t) = -\int_t^\infty dt'\, J(a,t'|x,0) \tag{5.2.177}$$

$$= \int_t^\infty dt' \{-A(a)p(a,t'|x,0) + \tfrac{1}{2}\partial_a[B(a)p(a,t'|x,0)]\} \tag{5.2.178}$$

(the negative sign is chosen since we need the current pointing to the left) and

$$g_b(x,t) = \int_t^\infty dt' \{A(b)p(b,t'|x,0) - \tfrac{1}{2}\partial_b[B(b)p(b,t'|x,0)]\}\,. \tag{5.2.179}$$

These 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

$$\text{Prob}(T_a > t) = g_a(x,t)/g_a(x,0)\,. \tag{5.2.180}$$

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

$$\begin{aligned} A(x)\partial_x g_a(x,t) + \tfrac{1}{2}B(x)\partial_x^2 g_a(x,t) &= -\int_t^\infty dt' \partial_{t'} J(a,t'|x,0) \\ &= J(a,t|x,0) \\ &= \partial_t g_a(x,t)\,. \end{aligned} \tag{5.2.181}$$

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

$$T(a,x) = -\int_0^\infty t\partial_t \text{Prob}\ (T_a > t)\, dt = \int_0^\infty g_a(x,t)dt/g_a(x,\infty)\,. \tag{5.2.182}$$

Simply integrating (5.2.181) with respect to t, we get

$$\boxed{A(x)\partial_x[\pi_a(x)T(a,x)] + \tfrac{1}{2}B(x)\partial_x^2[\pi_a(x)T(a,x)] = -\pi_a(x)\,,} \tag{5.2.183}$$

where we define

$$\pi_a(x) = (\text{probability of exit through } a) = g_a(x,0)\,. \tag{5.2.184}$$

The boundary conditions on (5.2.183) are quite straightforward since they follow from those for the backward Fokker-Planck equation, namely,

$$\pi_a(a)T(a,a) = \pi_a(b)T(a,b) = 0\,. \tag{5.2.185}$$

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 (5.2.181), 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

$$\boxed{A(x)\partial_x\pi_a(x) + \tfrac{1}{2}B(x)\partial_x^2\pi_a(x) = 0\,,} \tag{5.2.186}$$

the boundary condition this time being

$$\boxed{\begin{aligned} \pi_a(a) &= 1 \\ \pi_a(b) &= 0\,. \end{aligned}} \tag{5.2.187}$$

The solution of (5.2.186) subject to this boundary condition and the condition

$$\pi_a(x) + \pi_b(x) = 1 \tag{5.2.188}$$

is

$$\boxed{\pi_a(x) = [\int_x^b dy\, \psi(y)]/\int_a^b dy\, \psi(y)} \tag{5.2.189}$$

$$\boxed{\pi_b(x) = [\int_a^x dy\, \psi(y)]/\int_a^b dy\, \psi(y)} \tag{5.2.190}$$

with $\psi(x)$ as defined in (5.2.157).

These formulae find application in the problem of relaxation of a distribution initially concentrated at an unstable stationary point (Sect.9.1.4).

5.3 Fokker-Planck Equations in Several Dimensions

In many variable situations, Fokker-Planck equations take on an essentially more complex range of behaviour than is possible in the case of one variable. Boundaries are no longer simple end points of a line but rather curves or surfaces, and the nature of the boundary can change from place to place. Stationary solutions even with reflecting boundaries can correspond to nonzero probability currents and eigenfunction methods are no longer so simple.

Nevertheless, the analogies between one and many dimensions are useful, and this section will follow the same general outline as that on one-variable situations.

5.3.1 Change of Variables

Suppose we have a Fokker-Planck equation in variable x_i,

$$\partial_t p(\boldsymbol{x}, t) = -\sum_i \partial_i [A_i(\boldsymbol{x}) p(\boldsymbol{x}, t)] + \tfrac{1}{2} \sum_{i,j} \partial_i \partial_j [B_{ij}(\boldsymbol{x}) p(\boldsymbol{x}, t)] \tag{5.3.1}$$

and we want to know the corresponding equation for the variables

$$y_i = f_i(\boldsymbol{x}) , \tag{5.3.2}$$

where f_i are certain differentiable independent functions. Let us denote by $\bar{p}(\boldsymbol{y}, t)$ the probability density for the new variable, which is given by

$$\bar{p}(\boldsymbol{y}, t) = p(\boldsymbol{x}, t) \left| \frac{\partial(x_1, x_2 \ldots)}{\partial(y_1, y_2 \ldots)} \right| . \tag{5.3.3}$$

The simplest way to effect the change of variables is to use Ito's formula on the corresponding SDE

$$d\boldsymbol{x}(t) = A(\boldsymbol{x}) dt + \sqrt{\boldsymbol{B}(\boldsymbol{x})}\, d\boldsymbol{W}(t) \tag{5.3.4}$$

and then recompute the corresponding FPE for $\bar{p}(\boldsymbol{y}, t)$ from the resulting SDE as derived in Sect. 4.3.4.

The result is rather complicated. In specific situations, direct implementation (5.3.3) may be preferable. There is no way of avoiding a rather messy calculation unless full use of symmetries and simplifications is made.

Example: Cartesian to Polar Coordinates. As an example, one can consider the transformation to polar coordinates of the Rayleigh process, previously done by the SDE method in Sect.4.4.5. Thus, the Fokker-Planck equation is

$$\partial_t p(E_1, E_2, t) = \gamma \frac{\partial}{\partial E_1} E_1 p + \gamma \frac{\partial}{\partial E_2} E_2 p + \frac{1}{2} \varepsilon^2 \left(\frac{\partial^2 p}{\partial E_1^2} + \frac{\partial^2 p}{\partial E_2^2} \right) \tag{5.3.5}$$

and we want to find the FPE for a and ϕ defined by

$$\begin{aligned} E_1 &= a \cos\phi \\ E_2 &= a \sin\phi . \end{aligned} \tag{5.3.6}$$

The Jacobian is

$$\begin{aligned} |J| = \frac{\partial(E_1, E_2)}{\partial(a, \phi)} &= \begin{vmatrix} \cos\phi & -a \sin\phi \\ \sin\phi & a \cos\phi \end{vmatrix} \\ &= a . \end{aligned} \tag{5.3.7}$$

We use the polar form of the Laplacian to write

$$\frac{\partial^2}{\partial E_1^2} + \frac{\partial^2}{\partial E_2^2} = \frac{1}{a^2} \frac{\partial^2}{\partial \phi^2} + \frac{1}{a} \frac{\partial}{\partial a} \left(a \frac{\partial}{\partial a} \right) \tag{5.3.8}$$

and inverting (5.3.6)

$$\left.\begin{aligned} a &= \sqrt{E_1^2 + E_2^2} \\ \phi &= \tan^{-1}(E_2/E_1) , \end{aligned}\right\} \tag{5.3.9}$$

we note

$$\left.\begin{aligned} \frac{\partial a}{\partial E_1} &= \frac{E_1}{\sqrt{E_1^2 + E_2^2}} = \cos\phi . \\ &\text{Similarly,} \\ \frac{\partial a}{\partial E_2} &= \sin\phi \end{aligned}\right\} \tag{5.3.10}$$

and

$$\left.\begin{aligned} \frac{\partial \phi}{\partial E_2} &= \frac{E_1}{E_1^2 + E_2^2} = \cos\phi/a . \\ &\text{Similarly,} \\ \frac{\partial \phi}{\partial E_1} &= -\sin\phi/a . \end{aligned}\right\} \tag{5.3.11}$$

Hence,

$$\begin{aligned} &\frac{\partial}{\partial E_1} E_1 p + \frac{\partial}{\partial E_2} E_2 p \\ &\quad = 2p + E_1 \left(\frac{\partial p}{\partial a} \frac{\partial a}{\partial E_1} + \frac{\partial p}{\partial \phi} \frac{\partial \phi}{\partial E_1} \right) + E_2 \left(\frac{\partial p}{\partial a} \frac{\partial a}{\partial E_2} + \frac{\partial p}{\partial \phi} \frac{\partial \phi}{\partial E_2} \right) \\ &\quad = 2p + a \frac{\partial p}{\partial a} = \frac{1}{a} \frac{\partial}{\partial a} (a^2 p) . \end{aligned} \tag{5.3.12}$$

Let us use the symbol $\bar{p}(a, \phi)$ for the density function in terms of a and ϕ. The Jacobian formula (5.5.3) tells us that

$$\bar{p}(a, \phi) = \left| \frac{\partial(E_1, E_2)}{\partial(a, \phi)} \right| p(E_1, E_2) = a p(E_1, E_2) . \tag{5.3.13}$$

Putting together (5.3.5, 8, 12, 13), we get

$$\frac{\partial \bar{p}}{\partial t} = -\frac{\partial}{\partial a} \left[\left(-\gamma a + \frac{\varepsilon^2}{2a} \right) \bar{p} \right] + \frac{\varepsilon^2}{2} \left(\frac{1}{a^2} \frac{\partial^2 \bar{p}}{\partial \phi^2} + \frac{\partial^2 \bar{p}}{\partial a^2} \right) \tag{5.3.14}$$

which (of course) is the FPE, corresponding to the two SDE's in Sect.4.4.5, which were derived by changing variables according to Ito's formula.

5.3.2 Boundary Conditions

We have already touched on boundary conditions in general in Sect.5.2.1 where they were considered in terms of probability current. The full range of boundary conditions for an arbitrary multidimensional Fokker-Planck equation does not seem to have been specified yet. In this book we shall therefore consider mostly *reflecting barrier* boundary conditions at a surface $\boldsymbol{S}$, namely,

$$\boldsymbol{n}\cdot\boldsymbol{J}=0 \quad \text{on } \boldsymbol{S}, \tag{5.3.15}$$

where $\boldsymbol{n}$ is the normal to the surface and

$$J_i(\boldsymbol{x},t)=A_i(\boldsymbol{x},t)p(\boldsymbol{x},t)-\frac{1}{2}\sum_j\frac{\partial}{\partial x_j}B_{ij}(\boldsymbol{x},t)p(\boldsymbol{x},t) \tag{5.3.16}$$

and *absorbing barrier* boundary conditions

$$p(\boldsymbol{x},t)=0 \qquad \text{for } \boldsymbol{x} \text{ on } \boldsymbol{S}\,. \tag{5.3.17}$$

In practice, some part of the surface may be reflecting and another absorbing. At a surface $\boldsymbol{S}$ on which A_i or B_{ij} are discontinuous, we enforce

$$\begin{aligned}&\boldsymbol{n}\cdot\boldsymbol{J}_1=\boldsymbol{n}\cdot\boldsymbol{J}_2 \qquad \text{on } \boldsymbol{S}\\ &p_1(\boldsymbol{x})=p_2(\boldsymbol{x}) \qquad \boldsymbol{x} \text{ on } \boldsymbol{S}.\end{aligned} \tag{5.3.18}$$

The tangential current component is permitted to be discontinuous.

The boundary conditions on the backward equation have already been derived in Sect.5.2.4. For completeness, they are

$$\textit{Absorbing Boundary} \quad p(\boldsymbol{x},t|\boldsymbol{y},t')=0 \qquad \boldsymbol{y}\in\boldsymbol{S} \tag{5.3.19}$$

$$\textit{Reflecting Boundary} \quad \sum_{i,j}n_iB_{ij}(\boldsymbol{y})\frac{\partial}{\partial y_j}p(\boldsymbol{x},t|\boldsymbol{y},t')=0 \qquad \boldsymbol{y}\in\boldsymbol{S}\,. \tag{5.3.20}$$

5.3.3 Stationary Solutions: Potential Conditions

A large class of interesting systems is described by Fokker-Planck equations which permit a stationary distribution for which the probability current vanishes for all $\boldsymbol{x}$ in R. Assuming this to be the case, by rearranging the definition of $\boldsymbol{J}$ (5.3.16), we obtain a completely equivalent equation

$$\frac{1}{2}\sum_j B_{ij}(\boldsymbol{x})\frac{\partial p_s(\boldsymbol{x})}{\partial x_j}=p_s(\boldsymbol{x})\left[A_i(\boldsymbol{x})-\frac{1}{2}\sum_j\frac{\partial}{\partial x_j}B_{ij}(\boldsymbol{x})\right]. \tag{5.3.21}$$

If the matrix $B_{ij}(\boldsymbol{x})$ has an inverse for all $\boldsymbol{x}$, we can rewrite (5.3.21)

$$\frac{\partial}{\partial x_i}\log\left[p_s(\boldsymbol{x})\right]=\sum_k B^{-1}_{ik}(\boldsymbol{x})\left[2A_k(\boldsymbol{x})-\sum_j\frac{\partial}{\partial x_j}B_{kj}(\boldsymbol{x})\right] \tag{5.3.22}$$

$$\equiv Z_i[A,B,\boldsymbol{x}]\,. \tag{5.3.23}$$

This equation cannot be satisfied for arbitrary $B_{ij}(\boldsymbol{x})$ and $A_i(\boldsymbol{x})$ since the left-hand side is explicitly a gradient. Hence, Z_i must also be a gradient, and a necessary and sufficient condition for that is the vanishing of the curl, i.e.,

$$\frac{\partial Z_i}{\partial x_j}=\frac{\partial Z_j}{\partial x_i}. \tag{5.3.24}$$

If this condition is satisfied, the stationary solution can be obtained by simple integration of (5.3.22):

$$p_s(\boldsymbol{x})=\exp\left[\int^{\boldsymbol{x}}d\boldsymbol{x}'\cdot\boldsymbol{Z}[A,B,\boldsymbol{x}']\right]. \tag{5.3.25}$$

The conditions (5.3.24) are known as *potential conditions* since we derive the quantities Z_i from derivatives of $\log\left[p_s(\boldsymbol{x})\right]$, which, therefore, is often thought of as a potential $-\phi(\boldsymbol{x})$ so that more precisely,

$$p_s(\boldsymbol{x})=\exp\left[-\phi(\boldsymbol{x})\right] \tag{5.3.26}$$

and

$$\phi(\boldsymbol{x})=-\int^{\boldsymbol{x}}d\boldsymbol{x}'\cdot\boldsymbol{Z}[A,B,\boldsymbol{x}']\,. \tag{5.3.27}$$

Example: Rayleigh Process in Polar Coordinates. From (5.3.14) we find

$$\boldsymbol{A}=\begin{bmatrix}-\gamma a+\varepsilon^2/2a\\ 0\end{bmatrix} \tag{5.3.28}$$

$$\underline{\boldsymbol{B}}=\begin{bmatrix}\varepsilon^2 & 0\\ 0 & \varepsilon^2/a^2\end{bmatrix} \tag{5.3.29}$$

from which

$$\sum_j\frac{\partial}{\partial x_j}B_{a,j}=\sum_j\frac{\partial}{\partial x_j}B_{\phi,j}=0 \tag{5.3.30}$$

so that

$$\boldsymbol{Z}=2\,\underline{\boldsymbol{B}}^{-1}\boldsymbol{A}=\begin{bmatrix}-2\gamma a/\varepsilon^2+1/a\\ 0\end{bmatrix} \tag{5.3.31}$$

and clearly

$$\frac{\partial Z_a}{\partial \phi} = \frac{\partial Z_\phi}{\partial a} = 0 . \tag{5.3.32}$$

The stationary solution is then

$$p_s(a, \phi) = \exp[\int^{(a,\phi)} (d\phi\, Z_\phi + da\, Z_a)] \tag{5.3.33}$$

$$= \mathcal{N} \exp\left(-\frac{\gamma a^2}{\varepsilon^2} + \log a\right) \tag{5.3.34}$$

$$= \mathcal{N} a \exp\left(-\frac{\gamma a^2}{\varepsilon^2}\right). \tag{5.3.35}$$

5.3.4 Detailed Balance

a) Definition of Detailed Balance

The fact that the stationary solution of certain Fokker-Planck equations corresponds to a vanishing probability current is a particular version of the physical phenomenon of *detailed balance*. A Markov process satisfies detailed balance if, roughly speaking, in the stationary situation each possible transition balances with the reversed transition. The concept of detailed balance comes from physics, so let us explain more precisely with a physical example. We consider a gas of particles with positions $\boldsymbol{r}$ and velocities $\boldsymbol{v}$. Then a transition corresponds to a particle at some time t with position velocity $(\boldsymbol{r}, \boldsymbol{v})$ having acquired by a later time $t + \tau$ position and velocity $(\boldsymbol{r}', \boldsymbol{v}')$. The probability density of this transition is the *joint probability density* $p(\boldsymbol{r}', \boldsymbol{v}', t + \tau; \boldsymbol{r}, \boldsymbol{v}, t)$.

We may symbolically write this transition as

$$(\boldsymbol{r}, \boldsymbol{v}, t) \to (\boldsymbol{r}', \boldsymbol{v}', t + \tau) . \tag{5.3.36}$$

The reversed transition is not given simply by interchanging primed and unprimed quantities Rather, it is

$$(\boldsymbol{r}', -\boldsymbol{v}', t) \to (\boldsymbol{r}, -\boldsymbol{v}, t + \tau) . \tag{5.3.37}$$

It corresponds to the *time reversed transition* and requires the velocities to be reversed because the motion from $\boldsymbol{r}'$ to $\boldsymbol{r}$ is in the opposite direction from that from $\boldsymbol{r}$ to $\boldsymbol{r}'$.

The probability density for the reversed transition is thus the joint probability density

$$p(\boldsymbol{r}, -\boldsymbol{v}, t + \tau; \boldsymbol{r}', -\boldsymbol{v}', t) . \tag{5.3.38}$$

The *principle of detailed balance* requires the equality of these two joint probabilities when the system is in a stationary state. Thus, we may write

$$p_s(\boldsymbol{r}', \boldsymbol{v}', \tau; \boldsymbol{r}, \boldsymbol{v}, 0) = p_s(\boldsymbol{r}, -\boldsymbol{v}, \tau; \boldsymbol{r}', -\boldsymbol{v}', 0) \tag{5.3.39}$$

(The principle can be derived under certain conditions from the laws of physics, see [5.7] and Sect.5.3.6b.)

More explicitly, for a *Markov* process we can rewrite (5.3.39)

$$p(\boldsymbol{r}', \boldsymbol{v}', \tau | \boldsymbol{r}, \boldsymbol{v}, 0) p_s(\boldsymbol{r}, \boldsymbol{v}) = p(\boldsymbol{r}, -\boldsymbol{v}, \tau | \boldsymbol{r}', -\boldsymbol{v}', 0) p_s(\boldsymbol{r}', -\boldsymbol{v}') , \tag{5.3.40}$$

where the conditional probabilities now apply to the corresponding homogeneous Makov process (if the process was not Markov, the conditional probabilities would be for the stationary system only).

In its general form, detailed balance is formulated in terms of arbitrary variables x_i, which under time reversal, transform to the reversed variables according to the rule

$$x_i \to \varepsilon_i x_i \tag{5.3.41}$$

$$\varepsilon_i = \pm 1 \tag{5.3.42}$$

depending on whether the variable is odd or even under time reversal. In the above, $\boldsymbol{r}$ is even, $\boldsymbol{v}$ is odd.

Then by detailed balance we require

$$p_s(\boldsymbol{x}, t + \tau; \boldsymbol{x}', t) = p_s(\boldsymbol{\varepsilon x}', t + \tau; \boldsymbol{\varepsilon x}, t) . \tag{5.3.43}$$

By $\boldsymbol{\varepsilon x}$, we mean $(\varepsilon_1 x_1, \varepsilon_2 x_2, \ldots)$.

Notice that setting $\tau = 0$ in (5.3.43) we obtain

$$\delta(\boldsymbol{x} - \boldsymbol{x}') p_s(\boldsymbol{x}') = \delta(\boldsymbol{\varepsilon x} - \boldsymbol{\varepsilon x}') p_s(\boldsymbol{\varepsilon x}) . \tag{5.3.44}$$

The two delta functions are equal since only sign changes are involved. Hence,

$$p_s(\boldsymbol{x}) = p_s(\boldsymbol{\varepsilon x}) \tag{5.3.45}$$

is a consequence of the formulation of detailed balance by (5.3.43). Rewriting now in terms of conditional probabilities, we have

$$\boxed{p(\boldsymbol{x}, \tau | \boldsymbol{x}', 0) p_s(\boldsymbol{x}') = p(\boldsymbol{\varepsilon x}', \tau | \boldsymbol{\varepsilon x}, 0) p_s(\boldsymbol{x}) .} \tag{5.3.46}$$

b) General Consequences of Detailed Balance

An important consequence of (5.3.45) is that

$$\langle \boldsymbol{x} \rangle_s = \boldsymbol{\varepsilon} \langle \boldsymbol{x} \rangle_s \tag{5.3.47}$$

(hence all odd variables have zero stationary mean), and for the autocorrelation function

$$G(\tau) \equiv \langle \boldsymbol{x}(\tau) \boldsymbol{x}^{\mathrm{T}}(0) \rangle_s$$

we have

$$G(\tau) = \varepsilon \langle \boldsymbol{x}(0)\boldsymbol{x}^{\mathrm{T}}(\tau)\rangle_s \varepsilon ,$$

hence,

$$\boxed{G(\tau) = \varepsilon G^{\mathrm{T}}(\tau)\varepsilon} \tag{5.3.48}$$

and setting $\tau = 0$ and noting that the covariance matrix σ satisfies $\sigma = \sigma^{\mathrm{T}}$,

$$\sigma\varepsilon = \varepsilon\sigma . \tag{5.3.49}$$

For the spectrum matrix

$$S(\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}\omega\tau} G(\tau) ,$$

we find from (5.3.48) that

$$S(\omega) = \varepsilon S^{T}(\omega)\varepsilon . \tag{5.3.50}$$

c) Situations in Which Detailed Balance must be Generalised

It is possible that there exist several stationary solutions to a Markov process, and in this situation, a weaker form of detailed balance may hold, namely, instead of (5.3.43), we have

$$p_s^1(\boldsymbol{x}, t+\tau; \boldsymbol{x}', t) = p_s^2(\varepsilon\boldsymbol{x}', t+\tau; \varepsilon\boldsymbol{x}, t) \tag{5.3.51}$$

where the superscripts 1 and 2 refer to two different stationary solutions. Such a situation can exist if one of the variables is odd under time reversal, but does not change with time; for example, in a centrifuge the total angular momentum has this property. A constant magnetic field acts the same way.

Mostly, one writes the detailed balance conditions in such situations as

$$p_s^{\lambda}(\boldsymbol{x}, t+\tau; \boldsymbol{x}^1, t) = p_s^{\varepsilon\lambda}(\varepsilon\boldsymbol{x}', +\tau; \varepsilon\boldsymbol{x}, t) \tag{5.3.52}$$

where $\boldsymbol{\lambda}$ is a vector of such constant quantities, which change to $\varepsilon\boldsymbol{\lambda}$ under time reversal. According to one point of view, such a situation does not represent detailed balance; since in a given stationary situation, the transitions do *not* balance in detail. It is perhaps better to call the property (5.3.52) *time reversal invariance*.

In the remainder of our considerations, we shall mean by detailed balance the situation (5.3.45), since no strong consequences arise from the form (5.3.52).

5.3.5 Consequences of Detailed Balance

The formulation of detailed balance for the Fokker-Planck equation was done by *van Kampen* [5.7] and independently by *Uhlhorn* [5.8], and *Graham* and *Haken* [5.9]. We will formulate the conditions in a slightly more direct and more general way. We want necessary and sufficient conditions on the drift and diffusion coefficients and the jump probabilities for a homogeneous Markov process to have stationary solutions which satisfy detailed balance. We shall show that necessary and sufficient conditions are given by

$$\boxed{\begin{aligned} &\text{(i)} \quad W(\boldsymbol{x}|\boldsymbol{x}')p_s(\boldsymbol{x}') = W(\varepsilon\boldsymbol{x}'|\varepsilon\boldsymbol{x})p_s(\boldsymbol{x}) \\ &\text{(ii)} \quad \varepsilon_i A_i(\varepsilon\boldsymbol{x})p_s(\boldsymbol{x}) = -A_i(\boldsymbol{x})p_s(\boldsymbol{x}) + \sum_j \frac{\partial}{\partial x_j}[B_{ij}(\boldsymbol{x})p_s(\boldsymbol{x})] \\ &\text{(iii)} \quad \varepsilon_i\varepsilon_j B_{ij}(\varepsilon\boldsymbol{x}) = B_{ij}(\boldsymbol{x}) . \end{aligned}} \tag{5.3.53}$$

The specialisation to a FPE is simply done by setting the jump probabilities $W(\boldsymbol{x}|\boldsymbol{x}')$ equal to zero.

Necessary Conditions. It is simpler to formulate conditions for the differential Chapman-Kolmogorov equation than to restrict ourselves to the Fokker-Planck equation. According to Sect. 3.4 which defines the quantities $W(\boldsymbol{x}|\boldsymbol{x}')$, $A_i(\boldsymbol{x})$ and $B_{ij}(\boldsymbol{x})$ (all of course being time independent, since we are considering homogeneous process), we have the trivial result that detailed balance requires, from (5.3.46)

$$W(\boldsymbol{x}|\boldsymbol{x}')p_s(\boldsymbol{x}') = W(\varepsilon\boldsymbol{x}'|\varepsilon\boldsymbol{x})p_s(\boldsymbol{x}) . \tag{5.3.54}$$

Consider now the drift coefficient. For simplicity write

$$\boldsymbol{x}' = \boldsymbol{x} + \boldsymbol{\delta} . \tag{5.3.55}$$

Then from (5.3.46) we have

$$\begin{aligned} &\int_{|\delta|<K} d\boldsymbol{\delta}\, \delta_i p(\varepsilon\boldsymbol{x} + \varepsilon\boldsymbol{\delta}, \Delta t|\varepsilon\boldsymbol{x}, 0)p_s(\boldsymbol{x}) \\ &\quad = \int_{|\delta|<K} d\boldsymbol{\delta}\, \delta_i p(\boldsymbol{x}, \Delta t|\boldsymbol{x} + \boldsymbol{\delta}, 0)p_s(\boldsymbol{x} + \boldsymbol{\delta}) \end{aligned} \tag{5.3.56}$$

(we use K instead of ε in the range of integration to avoid confusion with ε_i); divide by Δt and take the limit $\Delta t \to 0$, and the left-hand side yields

$$\varepsilon_i A_i(\varepsilon\boldsymbol{x})p_s(\boldsymbol{x}) + O(K) . \tag{5.3.57}$$

On the right-hand side we write

$$\begin{aligned} p(\boldsymbol{x} + \boldsymbol{\delta} - \boldsymbol{\delta}, \Delta t|\boldsymbol{x} + \boldsymbol{\delta}, 0)p_s(\boldsymbol{x} + \boldsymbol{\delta}) &= p(\boldsymbol{x} - \boldsymbol{\delta}, \Delta t|\boldsymbol{x}, 0)p_s(\boldsymbol{x}) \\ &+ \sum_j \delta_j \frac{\partial}{\partial x_j}[p(\boldsymbol{x} - \boldsymbol{\delta}, \Delta t|\boldsymbol{x}, 0)p_s(\boldsymbol{x})] + O(\delta^2) \end{aligned} \tag{5.3.58}$$

so that the right-hand side is

$$\lim_{\Delta t\to 0}\frac{1}{\Delta t}\int d\boldsymbol{\delta}\left[\delta_i p(\boldsymbol{x}-\boldsymbol{\delta},\Delta t\,|\,\boldsymbol{x},0)p_s(\boldsymbol{x})+\sum_j \delta_i\delta_j\frac{\partial}{\partial x_j}[p(\boldsymbol{x}-\boldsymbol{\delta},\Delta t\,|\,\boldsymbol{x},0)p_s(\boldsymbol{x})]\right]+O(K)$$

$$=-A_i(\boldsymbol{x})p_s(\boldsymbol{x})+\sum_j\frac{\partial}{\partial x_j}[B_{ij}(\boldsymbol{x})p_s(\boldsymbol{x})]+O(K)\,, \tag{5.3.59}$$

where we have used the fact demonstrated in Sect. 3.4 that terms involving higher powers of δ than δ^2 are of order K. Letting $K\to 0$, we find

$$\varepsilon_i A_i(\varepsilon\boldsymbol{x})p_s(\boldsymbol{x})=-A_i(\boldsymbol{x})p_s(\boldsymbol{x})+\sum_j\frac{\partial}{\partial x_j}[B_{ij}(\boldsymbol{x})p_s(\boldsymbol{x})]\,. \tag{5.3.60}$$

The condition on $B_{ij}(\boldsymbol{x})$ is obtained similarly, but in this case no term like the second on the right of (5.3.60) arises, since the principal term is $O(\delta^2)$. We find

$$\varepsilon_i\varepsilon_j B_{ij}(\varepsilon\boldsymbol{x})=B_{ij}(\boldsymbol{x})\,. \tag{5.3.61}$$

A third condition is, of course, that $p_s(\boldsymbol{x})$ be a stationary solution of the differential Chapman-Kolmogorov equation. This is not a trivial condition, and is, in general, independent of the others.

Sufficient Conditions. We now show that (5.3.53) are sufficient. Assume that these conditions are satisfied, that $p_s(\boldsymbol{x})$ is a stationary solution of the differential Chapman-Kolmogorov equation, and that $p(\boldsymbol{x},t\,|\,\boldsymbol{x}',0)$ is a solution of the differential Chapman-Kolmogorov equation. We now consider a quantity

$$\hat{p}(\boldsymbol{x},t\,|\,\boldsymbol{x}',0)\equiv p(\varepsilon\boldsymbol{x}',t\,|\,\varepsilon\boldsymbol{x},0)p_s(\boldsymbol{x})/p_s(\boldsymbol{x}')\,. \tag{5.3.62}$$

Clearly

$$\hat{p}(\boldsymbol{x},0\,|\,\boldsymbol{x}',0)=\delta(\boldsymbol{x}-\boldsymbol{x}')=p(\boldsymbol{x},0\,|\,\boldsymbol{x}',0)\,. \tag{5.3.63}$$

We substitute $\hat{p}$ into the differential Chapman-Kolmogorov equation and show that because $p(\boldsymbol{x}',t\,|\,\boldsymbol{x},0)$ obeys the *backward differential Chapman-Kolmogorov equation* in the variable $\boldsymbol{x}$, the quantity $\hat{p}$ is a solution of the *forward differential Chapman-Kolmogorov equation*.

We do this explicitly. The notation is abbreviated for clarity, so that we write

$$\left.\begin{array}{lll}\hat{p} & \text{for} & \hat{p}(\boldsymbol{x},t\,|\,\boldsymbol{x}',0)\\ p_s & \text{for} & p_s(\boldsymbol{x})\\ p_s' & \text{for} & p_s(\boldsymbol{x}')\\ p(\boldsymbol{x}) & \text{for} & p(\boldsymbol{x}',t\,|\,\boldsymbol{x},0)\,.\end{array}\right\} \tag{5.3.64}$$

We proceed term by term.

i) **Drift Term**:

$$-\sum_i\frac{\partial}{\partial x_i}(A_i\hat{p})=-\sum_i\frac{\partial}{\partial x_i}(A_i p(\varepsilon\boldsymbol{x})p_s/p_s') \tag{5.3.65}$$

$$=-\sum_i\left[\frac{\partial}{\partial x_i}[A_i p_s]p(\varepsilon\boldsymbol{x})+A_i p_s\frac{\partial}{\partial x_i}p(\varepsilon\boldsymbol{x})\right]/p_s'\,.$$

ii) **Diffusion Term**:

$$\frac{1}{2}\sum_{i,j}\frac{\partial^2}{\partial x_i\partial x_j}(B_{ij}\hat{p})=\frac{1}{2}\sum_{i,j}\left[\frac{\partial^2}{\partial x_i\partial x_j}(B_{ij}p_s)p(\varepsilon\boldsymbol{x})\right.$$
$$\left.+2\frac{\partial}{\partial x_i}(B_{ij}p_s)\frac{\partial}{\partial x_j}p(\varepsilon\boldsymbol{x})+B_{ij}p_s\frac{\partial^2}{\partial x_i\partial x_j}p(\varepsilon\boldsymbol{x})\right]/p_s'\,. \tag{5.3.66}$$

iii) **Jump Term**:

$$\int d\boldsymbol{z}[W(\boldsymbol{x}\,|\,\boldsymbol{z})\hat{p}(\boldsymbol{z},t\,|\,\boldsymbol{x}',0)-W(\boldsymbol{z}\,|\,\boldsymbol{x})\hat{p}(\boldsymbol{x},t\,|\,\boldsymbol{x}',0)]$$
$$=\int d\boldsymbol{z}[W(\boldsymbol{x}\,|\,\boldsymbol{z})p_s(\boldsymbol{z})p(\varepsilon\boldsymbol{x}',t\,|\,\varepsilon\boldsymbol{z},0)-W(\boldsymbol{z}\,|\,\boldsymbol{x})p_s(\boldsymbol{x})p(\varepsilon\boldsymbol{x}',t\,|\,\varepsilon\boldsymbol{x},0)]/p_s\,. \tag{5.3.67}$$

We now use the fact that $p_s(\boldsymbol{x})$ is a solution of the stationary differential Chapman-Kolmogorov equation to write

$$-\sum_i\left[\frac{\partial}{\partial x_i}(A_i p_s)+\frac{1}{2}\sum_{i,j}\frac{\partial^2}{\partial x_i\partial x_i}(B_{ij}p_s)\right]-\int d\boldsymbol{z}\;W(\boldsymbol{z}\,|\,\boldsymbol{x})p_s(\boldsymbol{x})$$
$$=-\int d\boldsymbol{z}\;W(\boldsymbol{x}\,|\,\boldsymbol{z})p_s(\boldsymbol{z}) \tag{5.3.68}$$

and using the detailed balance condition (5.3.53(i)) for W

$$=-\int d\boldsymbol{z}\;W(\varepsilon\boldsymbol{z}\,|\,\varepsilon\boldsymbol{x})p_s(\boldsymbol{x})\,. \tag{5.3.69}$$

Now substitute

$$\begin{aligned}\boldsymbol{y}&=\varepsilon\boldsymbol{x}\\ \boldsymbol{y}'&=\varepsilon\boldsymbol{x}'\end{aligned} \tag{5.3.70}$$

and all up all three contributions, taking care of (5.3.68, 69):

$$=\left\{-\sum_i\varepsilon_i A_i(\varepsilon\boldsymbol{y})p_s(\boldsymbol{y})\left[\frac{\partial}{\partial y_i}p(\boldsymbol{y})\right]+\sum_{i,j}\varepsilon_i\varepsilon_j\frac{\partial}{\partial y_j}[B_{ij}(\varepsilon\boldsymbol{y})p_s(\boldsymbol{y})]\left[\frac{\partial}{\partial y_i}p(\boldsymbol{y})\right]\right.$$
$$+\frac{1}{2}\sum_{i,j}\varepsilon_i\varepsilon_j B_{ij}(\varepsilon\boldsymbol{y})p_s(\boldsymbol{y})\left[\frac{\partial^2}{\partial y_i\partial y_j}p(\boldsymbol{y})\right] \tag{5.3.71}$$
$$\left.+\int d\boldsymbol{z}[W(\varepsilon\boldsymbol{y}\,|\,\boldsymbol{z})p_s(\boldsymbol{z})p(\boldsymbol{y}',t\,|\,\varepsilon\boldsymbol{z},0)-W(\varepsilon\boldsymbol{y}\,|\,\boldsymbol{z})p_s(\boldsymbol{z})p(\boldsymbol{y}',t\,|\,\boldsymbol{y},0)]\right|/p_s(\boldsymbol{y}').$$

We now substitute the detailed balance conditions (5.3.53).

$$=\left[\sum_i A_i(\boldsymbol{y})\frac{\partial}{\partial y_i}p(\boldsymbol{y}',t\,|\,\boldsymbol{y},0)+\frac{1}{2}\sum_{i,j}B_{ij}(\boldsymbol{y})\frac{\partial^2}{\partial y_i\partial y_j}p(\boldsymbol{y}',t\,|\,\boldsymbol{y},0)\right.$$
$$\left.+\int d\boldsymbol{z}[W(\boldsymbol{z}\,|\,\boldsymbol{y})p(\boldsymbol{y}',t\,|\,\boldsymbol{z},0)-W(\boldsymbol{z}\,|\,\boldsymbol{y})p(\boldsymbol{y}',t\,|\,\boldsymbol{y},0)\right]p_s(\boldsymbol{y})/p_s(\boldsymbol{y}')\,. \tag{5.3.72}$$

The term in the large curly brackets is now recognisable as the *backward differential Chapman-Kolmogorov operator* [Sect.3.6, (3.6.4)]. Note that the process is homogeneous, so that

$$p(\boldsymbol{y}', t|\boldsymbol{y}, 0) = p(\boldsymbol{y}, 0|\boldsymbol{y}, -t)\,.$$

We see that

$$(5.3.72) = \frac{\partial}{\partial t}[p(\boldsymbol{y}', t|, 0)p_s(\boldsymbol{y})/p_s(\boldsymbol{y}')] = \frac{\partial}{\partial t}\hat{p}(\boldsymbol{x}, t|\boldsymbol{x}', 0) \tag{5.3.73}$$

which means that $\hat{p}(\boldsymbol{x}, t|\boldsymbol{x}', 0)$, defined in (5.3.62), satisfies the forward differential Chapman-Kolmogorov equation. Since the initial condition of $p(\boldsymbol{x}, t|\boldsymbol{x}', 0)$ and $\hat{p}(\boldsymbol{x}, t|\boldsymbol{x}', 0)$ at $t = 0$ are the same (5.3.63) and the solutions are unique, we have shown that provided the detailed balance conditions (5.3.53) are satisfied, detailed balance is satisfied. Hence, sufficiency is shown.

Comments

i) *Even variables only*: the conditions are considerably simpler if all ε_i are $+1$. In this case, the conditions reduce to

$$W(\boldsymbol{x}|\boldsymbol{x}')p_s(\boldsymbol{x}') = W(\boldsymbol{x}'|\boldsymbol{x})p_s(\boldsymbol{x}) \tag{5.3.74}$$

$$A_i(\boldsymbol{x})p_s(\boldsymbol{x}) = \frac{1}{2}\sum_j \frac{\partial}{\partial x_j}[B_{ij}(\boldsymbol{x})p_s(\boldsymbol{x})] \tag{5.3.75}$$

$$B_{ij}(\boldsymbol{x}) = B_{ij}(\boldsymbol{x})\,, \tag{5.3.76}$$

the last of which is trivial. The condition (5.3.75) is exactly the same as the potential condition (5.3.21) which expresses the vanishing of $\boldsymbol{J}$, the probability current in the stationary state.

The conditions (5.3.74, 75) taken together imply that $p_s(\boldsymbol{x})$ satisfies the stationary differential Chapman-Kolmogorov equation, which is not the case for the general conditions (5.3.53).

ii) *Fokker-Planck equations*: *van Kampen*, [5.7], and *Graham* and *Haken* [5.9] introduced the concept of reversible and irreversible drift parts. The irreversible drift is

$$D_i(\boldsymbol{x}) = \tfrac{1}{2}[A_i(\boldsymbol{x}) + \varepsilon_i A_i(\varepsilon\boldsymbol{x})] \tag{5.3.77}$$

and the reversible drift

$$I_i(\boldsymbol{x}) = \tfrac{1}{2}[A_i(\boldsymbol{x}) - \varepsilon_i A_i(\varepsilon\boldsymbol{x}]\,. \tag{5.3.78}$$

Using again the potential defined by

$$p_s(\boldsymbol{x}) = \exp[-\phi(\boldsymbol{x})]\,, \tag{5.3.79}$$

we see that in the case of a Fokker-Planck equation, we can write the conditions for detailed balance as

$$\varepsilon_i\varepsilon_j B_{ij}(\varepsilon\boldsymbol{x}) = B_{ij}(\boldsymbol{x}) \tag{5.3.80}$$

$$D_i(\boldsymbol{x}) - \frac{1}{2}\sum_j \frac{\partial}{\partial x_j}[B_{ij}(\boldsymbol{x})] = -\frac{1}{2}\sum_i B_{ij}(\boldsymbol{x})\frac{\partial\phi(\boldsymbol{x})}{\partial x_j} \tag{5.3.81}$$

$$\sum_i \left[\frac{\partial}{\partial x_i} I_i(\boldsymbol{x}) - I_i(\boldsymbol{x})\frac{\partial\phi(\boldsymbol{x})}{\partial x_i}\right] = 0 \tag{5.3.82}$$

where the last equation is simply the stationary FPE for $p_s(\boldsymbol{x})$, after substituting (3.3.53(i)). As was the case for the potential conditions, it can be seen that (5.3.81) gives an equation for $\partial\phi/\partial x_j$ which can only be satisfied provided certain conditions on $D_i(\boldsymbol{x})$ and $B_{ij}(\boldsymbol{x})$ are satisfied. If $B_{ij}(\boldsymbol{x})$ has an inverse, these take the form

$$\frac{\partial\hat{Z}_i}{\partial x_j} = \frac{\partial\hat{Z}_j}{\partial x_i}\,, \tag{5.3.83}$$

where

$$\hat{Z}_i = \sum_k B^{-1}_{ik}(\boldsymbol{x})\left[2D_k(\boldsymbol{x}) - \sum_j \frac{\partial}{\partial x_j} B_{kj}(\boldsymbol{x})\right] \tag{5.3.84}$$

and we have

$$p_s(\boldsymbol{x}) = \exp[-\phi(\boldsymbol{x})] = \exp\left(\int^{\boldsymbol{x}} d\boldsymbol{x}'\cdot\hat{\boldsymbol{Z}}\right). \tag{5.3.85}$$

Thus, as in the case of a vanishing probability current, $p_s(\boldsymbol{x})$ can be determined explicitly as an integral.

iii) *Connection between backward and forward operators* of differential Chapman-Kolmogorov equations is provided by the detailed balance. The proof of sufficient conditions amounts to showing that if $f(\boldsymbol{x}, t)$ is a solution of the forward differential Chapman-Kolmogorov equation, then

$$\tilde{f}(\boldsymbol{x}, t) = f(\varepsilon\boldsymbol{x}, -t)/p_s(\boldsymbol{x}) \tag{5.3.86}$$

is a solution of the backward differential Chapman-Kolmogorov equation. This relationship will be used in Sect.5.3.7 for the construction of eigenfunctions.

5.3.6 Examples of Detailed Balance in Fokker-Planck Equations

a) Kramers' Equation for Brownian Motion [5.10]

We take the motion of a particle in a fluctuating environment. The motion is in one dimension and the state of the particle is described by its position x and velocity v. This gives the differential equations

$$\frac{dx}{dt} = v \tag{5.3.87}$$

and

$$m\frac{dv}{dt} = -V'(x) - \beta v + \sqrt{2\beta kT}\,\xi(t) \tag{5.3.88}$$

which are essentially Langevin's equations (1.2.14) in which for brevity, we write

$$6\pi\eta a = \beta$$

and $V(x)$ is a potential whose gradient $V'(x)$ gives rise to a force on the particle. By making the assumption that the physical fluctuating force $\xi(t)$ is to be interpreted as

$$\xi(t)dt = dW(t) \tag{5.3.89}$$

as explained in Sect.4.1, we obtain SDE's

$$dx = v\ dt \tag{5.3.90}$$

$$m\ dv = -[V'(x) + \beta v]\,dt + \sqrt{2\beta\, kT}\,dW(t) \tag{5.3.91}$$

for which the corresponding FPE is

$$\frac{\partial p}{\partial t} = -\frac{\partial}{\partial x}(vp) + \frac{1}{m}\frac{\partial}{\partial v}\{[V'(x) + \beta v]p\} + \frac{\beta\, kT}{m^2}\frac{\partial^2 p}{\partial v^2}. \tag{5.3.92}$$

The equation can be slightly simplified by introducing new scaled variables

$$y = x\sqrt{m/kT} \tag{5.3.93}$$

$$u = v\sqrt{m/kT} \tag{5.3.94}$$

$$U(y) = V(x)/kT \tag{5.3.95}$$

$$\gamma = \beta/m \tag{5.3.96}$$

so that the FPE takes the form

$$\frac{\partial p}{\partial t} = -\frac{\partial}{\partial y}(up) + \frac{\partial}{\partial u}[U'(y)p] + \gamma\frac{\partial}{\partial u}\left(up + \frac{\partial p}{\partial u}\right) \tag{5.3.97}$$

which we shall call *Kramers' equation*.

Here, y (the position) is an even variable and u (the velocity) an odd variable, as explained in Sect.5.3.4. The drift and diffusion can be written

$$\boldsymbol{A}(y, u) = \begin{bmatrix} u \\ -U'(y) - \gamma u \end{bmatrix}, \tag{5.3.98}$$

$$\boldsymbol{B}(y, u) = \begin{bmatrix} 0 & 0 \\ 0 & 2\gamma \end{bmatrix} \tag{5.3.99}$$

and

$$\boldsymbol{\varepsilon}\begin{bmatrix} y \\ u \end{bmatrix} = \begin{bmatrix} y \\ -u \end{bmatrix}. \tag{5.3.100}$$

We can check the conditions one by one.

The condition (5.3.53(iii)) is trivially satisfied. The condition (5.3.53(ii)) is somewhat degenerate, since $\boldsymbol{B}$ is not invertible. It can be written

$$\boldsymbol{\varepsilon A}(y, -u)p_s(y, u) = -\boldsymbol{A}(y, u)p_s(y, u) + \begin{bmatrix} 0 \\ 2\gamma\dfrac{\partial p_s}{\partial u} \end{bmatrix} \tag{5.3.101}$$

or, more fully

$$\begin{bmatrix} -u \\ U'(y) - \gamma u \end{bmatrix} p_s = \begin{bmatrix} -u \\ U'(y) + \gamma u \end{bmatrix} p_s + \begin{bmatrix} 0 \\ 2\gamma\dfrac{\partial p_s}{\partial u} \end{bmatrix}. \tag{5.3.102}$$

The first line is an identity and the second states

$$-up_s(y, u) = \frac{\partial p_s}{\partial u}, \tag{5.3.103}$$

i.e.,

$$p_s(y, u) = \exp(-\tfrac{1}{2}u^2)f(y) \tag{5.3.104}$$

which means that if $p_s(y, u)$ is written in the form (5.3.104), then the detailed balance conditions are satisfied. One must now check whether (5.3.104) indeed gives a stationary solution of Kramers' equation (5.3.97) by substitution. The final bracket vanishes, leaving

$$0 = -u\frac{\partial f}{\partial y} - U'(y)uf \tag{5.3.105}$$

which means

$$f(y) = \mathcal{N}\exp[-U(y)] \tag{5.3.106}$$

and

$$p_s(y, u) = \mathcal{N} \exp\left[-U(y) - \tfrac{1}{2}u^2\right] . \tag{5.3.107}$$

In terms of the original (x, v) variables,

$$p_s(x, v) = \mathcal{N} \exp\left[-\frac{V(x)}{kT} - \frac{mv^2}{2kT}\right] \tag{5.3.108}$$

which is the familiar Boltzmann distribution of statistical mechanics. Notice that the denominators kT arise from the assumed coefficient $\sqrt{2\beta kT}$ of the fluctuating force in (5.3.88). Thus, we take the macroscopic equations and add a fluctuating force, whose magnitude is fixed by the requirement that the solution be the Boltzmann distribution corresponding to the temperature T.

But we have also achieved exactly the right distribution function. This means that the assumption that Brownian motion is described by a *Markov* process of the form (5.3.87, 88) must have considerable validity.

b) Deterministic Motion

Here we have $B_{ij}(\boldsymbol{x})$ and $W(\boldsymbol{x}|\boldsymbol{x}')$ equal to zero, so the detailed balance conditions are simply

$$\varepsilon_i A_i(\varepsilon \boldsymbol{x}) = -A_i(\boldsymbol{x}) . \tag{5.3.109}$$

Since we are now dealing with a Liouville equation (Sect.3.5.3), the motion of a point whose coordinates are $\boldsymbol{x}$ is described by the ordinary differential equation

$$\frac{d}{dt}\boldsymbol{x}(t) = \boldsymbol{A}[\boldsymbol{x}(t)] . \tag{5.3.110}$$

Suppose a solution of (5.3.110) which passes through the point $\boldsymbol{y}$ at $t = 0$ is

$$\boldsymbol{q}[t, \boldsymbol{y}] \tag{5.3.111}$$

which therefore satisfies

$$\boldsymbol{q}[0, \boldsymbol{y}] = \boldsymbol{y} . \tag{5.3.112}$$

Then the relation (5.3.109) implies that the reversed solution

$$\varepsilon \boldsymbol{q}(-t, \varepsilon \boldsymbol{y}) \tag{5.3.113}$$

is also a solution of (5.3.110), and since

$$\varepsilon \boldsymbol{q}(0, \varepsilon \boldsymbol{y}) = \varepsilon\varepsilon \boldsymbol{y} = \boldsymbol{y} , \tag{5.3.114}$$

i.e., the initial conditions are the same, these solutions must be identical, i.e.,

$$\varepsilon \boldsymbol{q}(-t, \varepsilon \boldsymbol{y}) = \boldsymbol{q}(t, \boldsymbol{y}) . \tag{5.3.115}$$

Now the joint probability in the stationary state can be written as

$$p_s(\boldsymbol{x}, t; \boldsymbol{x}', t') = \int d\boldsymbol{y}\, p_s(\boldsymbol{x}, t; \boldsymbol{x}', t'; \boldsymbol{y}, 0)$$
$$= \int d\boldsymbol{y}\, \delta[\boldsymbol{x} - \boldsymbol{q}(t, \boldsymbol{y})]\delta[\boldsymbol{x}' - \boldsymbol{q}(t', \boldsymbol{y})] p_s(\boldsymbol{y}) \tag{5.3.116}$$

and

$$p_s(\varepsilon \boldsymbol{x}', -t'; \varepsilon \boldsymbol{x}, -t) = \int d\boldsymbol{y}\, \delta[\varepsilon \boldsymbol{x} - \boldsymbol{q}(-t, \boldsymbol{y})]\delta[\varepsilon \boldsymbol{x}' - \boldsymbol{q}(-t', \boldsymbol{y})] p_s(\boldsymbol{y}) . \tag{5.3.117}$$

Change the variables from $\boldsymbol{y}$ to $\varepsilon \boldsymbol{y}$ and note that $p_s(\boldsymbol{y}) = p_s(\varepsilon \boldsymbol{y})$, and $d\varepsilon \boldsymbol{y} = d\boldsymbol{y}$, so that

$$(5.3.117) = \int d\boldsymbol{y}\, \delta[\boldsymbol{x} - \varepsilon \boldsymbol{q}(-t, \varepsilon \boldsymbol{y})]\delta[\boldsymbol{x}' - \varepsilon \boldsymbol{q}(-t', \varepsilon \boldsymbol{y})] p_s(\boldsymbol{y}) \tag{5.3.118}$$

and using (5.3.115),

$$= \int d\boldsymbol{y}\, \delta[\boldsymbol{x} - \boldsymbol{q}(t, \boldsymbol{y})]\delta[\boldsymbol{x}' - \boldsymbol{q}(t', \boldsymbol{y})] p_s(\boldsymbol{y}) \tag{5.3.119}$$
$$= p_s(\boldsymbol{x}, t; \boldsymbol{x}', t') . \tag{5.3.120}$$

Using the stationarity property, that p_s depends only on the time difference, we see that detailed balance is satisfied.

This direct proof is, of course, unnecessary since the original general proof is valid for this deterministic system. Furthermore, any system of deterministic first-order differential equations can be transformed into a Liouville equation, so this direct proof is in general unnecessary and it is included here merely as a matter of interest.

However, it is important to give a brief summary of the philosophy behind this demonstration of detailed balance. In physical systems, which are where detailed balance is important, we often have an unbelievably large number of variables, of the order of 10^{20} at least. These variables (say, momentum and velocity of the particles in a gas) are those which occur in the distribution function which obeys a Liouville equation for they follow deterministic equations of motion, like Newton's laws of motion.

It can be shown directly that, for appropriate forms of interaction, Newton's laws obey the principle of *microscopic reversibility* which means that they can be put in the form (5.3.110), where $\boldsymbol{A}(\boldsymbol{x})$ obeys the reversibility condition (5.3.109).

The macroscopically observable quantities in such a system are functions of these variables (for example, pressure, temperature, density of particles) and, by appropriate changes of variable, can be represented by the first few components of the vector $\boldsymbol{x}$.

Thus, we assume $\boldsymbol{x}$ can be written

$$\boldsymbol{x} = (\boldsymbol{a}, \hat{\boldsymbol{x}}) \tag{5.3.121}$$

where the vector $\boldsymbol{a}$ represents the macroscopically observable quantities and $\hat{\boldsymbol{x}}$ is all the others. Then, in practice, we are interested in

$$p(\boldsymbol{a}_1, t_1; \boldsymbol{a}_2, t_2; \boldsymbol{a}_3, t_3; \ldots)$$
$$= \int\int \ldots \int d\hat{\boldsymbol{x}}_1, d\hat{\boldsymbol{x}}_2 \ldots p(\boldsymbol{x}_1, t_1; \boldsymbol{x}_2, t_2; \boldsymbol{x}_3, t_3; \ldots) . \tag{5.3.122}$$