5. Fokker-Planck Equation for One Variable; Methods of Solution

We now want to discuss methods for solving the one-variable Fokker-Planck equation (4.44, 45) with time-independent drift and diffusion coefficients, assuming $D^{(2)}(x) > 0$

$$\partial W(x,t)/\partial t = \boldsymbol{L}_{\mathrm{FP}} W(x,t) = -(\partial/\partial x) S(x,t), \tag{5.1}$$

$$L_{\mathrm{FP}}(x) = -\frac{\partial}{\partial x} D^{(1)}(x) + \frac{\partial^2}{\partial x^2} D^{(2)}(x). \tag{5.2}$$

In (5.1) S is the probability current (4.47).

The stochastic Langevin equation (3.67), for instance, with Gaussian δ-correlated Langevin forces and time-independent h and g leads to (5.1, 2) with $D^{(2)}(x)$ and $D^{(1)}(x)$ given by (3.95).

The Smoluchowski equation (1.23) describing one-dimensional Brownian motion of a particle in the potential $f(x)$ in the high-friction limit is a special case of (5.1, 2), where the drift and diffusion coefficients are given by

$$D^{(1)} = (m\gamma)^{-1} F(x) = -(m\gamma)^{-1} \tilde{f}'(x), \tag{5.3}$$

$$D^{(2)} = kT(m\gamma)^{-1}. \tag{5.4}$$

In (5.3) $F(x) = -\tilde{f}'(x)$ is the force due to the potential $\tilde{f}(x)$, m is the mass of the particle, γ is the friction constant, k is Boltzmann's constant and T is the temperature of the surrounding heat bath. The derivation of this Smoluchowski equation from the two-variable Fokker-Planck equation in position and velocity space (i.e., Kramers equation) is discussed in detail in Sect. 10.4.

5.1 Normalization

By a suitable transformation $x' \equiv y = y(x)$ the x-dependent diffusion coefficient can be transformed to an arbitrary constant $D > 0$. For the one-variable case this transformation according to (4.132) reads

$$D'^{(2)} \equiv D = \left(\frac{\mathrm{d}y}{\mathrm{d}x}\right)^2 D^{(2)}(x). \tag{5.5}$$

Thus this transformation is given by

$$y = y(x) = \int_{x_0}^{x} \sqrt{D/D^{(2)}(\xi)}\, \mathrm{d}\xi. \tag{5.6}$$

The transformed drift coefficient then takes the form [see (4.131)]

$$\begin{aligned} D'^{(1)}(y) &= \frac{\mathrm{d}y}{\mathrm{d}x} D^{(1)}(x) + \frac{\mathrm{d}^2 y}{\mathrm{d}x^2} D^{(2)}(x) \\ &= \sqrt{\frac{D}{D^{(2)}(x)}} \left[D^{(1)}(x) - \frac{1}{2} \frac{\mathrm{d}D^{(2)}(x)}{\mathrm{d}x} \right] \end{aligned} \tag{5.7}$$

and the transformed Fokker-Planck equation reads (D = const)

$$\frac{\partial W'(y,t)}{\partial t} = \left[-\frac{\partial}{\partial y} D'^{(1)}(y) + D \frac{\partial^2}{\partial y^2} \right] W'(y,t), \tag{5.8}$$

where W' is given by, cf. (4.119),

$$W' = J \cdot W = (\mathrm{d}y/\mathrm{d}x)^{-1} W = \sqrt{D^{(2)}(x)/D}\, W. \tag{5.9}$$

In (5.7 and 9) $x = x(y)$ has to be expressed by the y variable according to (5.6). Without loss of generality we may thus treat the equation with constant diffusion coefficient, i.e.,

$$\frac{\partial W}{\partial t} = \left[\frac{\partial}{\partial x} f'(x) + D \frac{\partial^2}{\partial x^2} \right] W = -\frac{\partial}{\partial x} S(x,t), \tag{5.10}$$

where S is the probability current.

Here we have introduced the potential

$$f(x) = -\int^{x} D^{(1)}(x')\, \mathrm{d}x'. \tag{5.11}$$

Up to a constant the potential (5.11) agrees with the potential $\tilde{f}$ of the Smoluchowski equation.

Because D is arbitrary, we may use $D = 1$. This normalization is, however, not very convenient if the low-noise limit $D \to 0$ is considered and we therefore retain the constant D.

Transformation (5.6) can also be done in the Langevin equation, see (3.69, 70, 95).

5.2 Stationary Solution

For stationary solutions the probability current in (5.1) must be constant. Thus, if the probability current vanishes at some x the current must be zero for any x. Then for $S = 0$

$$D^{(1)}(x)\, W_{\mathrm{st}}(x) = \frac{D^{(1)}(x)}{D^{(2)}(x)} D^{(2)}(x)\, W_{\mathrm{st}}(x) = \frac{\partial}{\partial x} D^{(2)}(x)\, W_{\mathrm{st}}(x)\,. \tag{5.12}$$

We can immediately integrate (5.12), yielding

$$W_{\mathrm{st}}(x) = \frac{N_0}{D^{(2)}(x)} \exp\left(\int^x \frac{D^{(1)}(x')}{D^{(2)}(x')}\, \mathrm{d}x' \right) = N \mathrm{e}^{-\Phi(x)}\,, \tag{5.13}$$

where N_0 is the integration constant, which has to be chosen such that W_{st} is normalized. In (5.13) we introduced the potential

$$\Phi(x) = \ln D^{(2)}(x) - \int^x \frac{D^{(1)}(x')}{D^{(2)}(x')}\, \mathrm{d}x'\,. \tag{5.14}$$

For the case of the Smoluchowski equation (5.3, 4) we may put $\Phi(x) = \tilde{f}(x)/(kT)$ and for (5.10) $\Phi(x) = f(x)/D$ because the potential $\Phi(x)$ is defined only up to an additive constant and therefore the $\ln D^{(2)}$ term may be omitted. Introducing this potential the probability current may be written in the form

$$S(x,t) = -D^{(2)}(x)\, \mathrm{e}^{-\Phi(x)} \frac{\partial}{\partial x} \left[\mathrm{e}^{\Phi(x)} W(x,t) \right]. \tag{5.15}$$

In the stationary state, where S is constant, we thus have for arbitrary S

$$W_{\mathrm{st}}(x) = N \mathrm{e}^{-\Phi(x)} - S \mathrm{e}^{-\Phi(x)} \int^x \frac{\mathrm{e}^{\Phi(x')}}{D^{(2)}(x')}\, \mathrm{d}x'\,. \tag{5.16}$$

One of the integration constants in (5.16) is determined by the normalization

$$\int W_{\mathrm{st}}(x)\, \mathrm{d}x = 1\,, \tag{5.17}$$

the other constant must be determined from the boundary conditions, so the problem arises as to which boundary conditions must be used. (For a further discussion of boundary conditions, see Sect. 5.4.) For problems where x extends to $\pm\infty$, we require that the integral (5.17) exists. In that case, W and also S must vanish at $\pm\infty$ (natural boundary conditions) and therefore $S = 0$ for every x. If the stochastic variable ξ cannot reach values smaller than $x_{\min}$, we require that the probability current must be zero at $x_{\min}$. In the stationary state, S then also vanishes for every x, i.e., (5.16) reduces to (5.13). There may, of course, also be other boundary conditions. If for instance x is an angle variable we usually require that the distribution function is periodic. In that case, S is determined by this periodicity condition. The current will then be zero only if $f(x)$ is also periodic. For a further discussion of boundary conditions, see Sect. 5.4.

An important question is whether every initial distribution finally decays to the stationary distribution. For some restrictions of the drift and diffusion coefficients and of the boundary conditions one can prove that any two solutions of the Fokker-Planck equation agree for large times. Thus if a stationary solution exists, every solution must finally decay to that solution. We postpone the derivation of the proof to Sect. 6.1, where a proof is given for the general N-variable case. We further show in Sect. 5.4 that all eigenvalues with the exception of the stationary eigenvalue $\lambda = 0$ are larger than zero, which also answers the above question positively.

5.3 Ornstein-Uhlenbeck Process

Nonstationary solutions of the Fokker-Planck equation (5.1, 2) are more difficult to obtain. A general expression for the nonstationary solution can be found only for special drift and diffusion coefficients.

Wiener Process

A process which is described by (5.1, 2) with vanishing drift coefficient ($D^{(1)} = 0$) and constant diffusion coefficient $D^{(2)}(x) = D$ is called a Wiener process. The equation for the transition probability $P = P(x, t \mid x', t')$ is then the diffusion equation

$$\frac{\partial P}{\partial t} = D \frac{\partial^2 P}{\partial x^2} \tag{5.18}$$

with the initial condition

$$P(x, t' | x', t') = \delta(x - x')\,. \tag{5.19}$$

The solution for $t > t'$ reads [5.1]

$$P(x, t | x', t') = \frac{1}{\sqrt{4\pi D(t-t')}} \exp\left(-\frac{(x-x')^2}{4D(t-t')} \right). \tag{5.20}$$

The general solution for the probability density with the initial distribution $W(x', t')$ is then given by

$$W(x,t) = \int P(x, t | x', t')\, W(x', t')\, \mathrm{d}x'\,. \tag{5.21}$$

Thus the transition probability serves as the Green's function of (5.18).

For the Ornstein-Uhlenbeck process the drift coefficient is linear and the diffusion coefficient is constant, i.e.,

Ornstein-Uhlenbeck Process

$$D^{(1)}(x) = -\gamma x\,; \quad D^{(2)}(x) = D = \text{const}\,. \tag{5.22}$$

With these coefficients the Fokker-Planck equation is the same as the Smoluchowski equation for a harmonically bound oscillator. In this case $\gamma = \omega_0^2/m$ is positive.

The equation for the transition probability now reads

$$\frac{\partial P}{\partial t} = \gamma \frac{\partial}{\partial x}(xP) + D\frac{\partial^2}{\partial x^2}P \tag{5.23}$$

with the initial condition (5.19). The solution of (5.23) is best found by making a Fourier transform with respect to x, i.e.,

$$P(x,t\,|x',t') = (2\pi)^{-1}\int \mathrm{e}^{\mathrm{i}kx}\tilde{P}(k,t\,|x',t')\,\mathrm{d}k\,. \tag{5.24}$$

The equation for the Fourier transform is given by (replace $\partial/\partial x$ by $\mathrm{i}k$ and x by $\mathrm{i}\partial/\partial k$)

$$\frac{\partial \tilde{P}}{\partial t} = -\gamma k\frac{\partial}{\partial k}\tilde{P} - Dk^2\tilde{P}\,, \tag{5.25}$$

which is simpler than (5.23) because only first-order derivatives with respect to k occur. Because of (5.19) the initial condition for the Fourier transform is

$$\tilde{P}(k,t'\,|x',t') = \mathrm{e}^{-\mathrm{i}kx'}\,. \tag{5.26}$$

The first-order equation (5.25) may be solved by the methods of characteristics [5.1]. The solution of (5.25) with the initial condition (5.26) reads ($t > t'$)

$$\tilde{P}(k,t\,|x',t') = \exp[-\mathrm{i}kx'\mathrm{e}^{-\gamma(t-t')} - Dk^2(1-\mathrm{e}^{-2\gamma(t-t')})/(2\gamma)]\,, \tag{5.27}$$

as may easily be checked by insertion. By performing the integral in (5.24) [cf. (2.32)] we finally get the Gaussian distribution ($t > t'$)

$$P(x,t\,|x',t') = \sqrt{\frac{\gamma}{2\pi D(1-\mathrm{e}^{-2\gamma(t-t')})}}\exp\left[-\frac{\gamma(x-\mathrm{e}^{-\gamma(t-t')}x')^2}{2D(1-\mathrm{e}^{-2\gamma(t-t')})}\right]. \tag{5.28}$$

In the limit $\gamma \to 0$ we recover the result (5.20) for the Wiener process.

Equation (5.28) is valid for positive and negative γ. For positive γ and large time differences $\gamma(t-t') \gg 1$, (5.28) passes over to the stationary distribution

$$W_{\mathrm{st}}(x) = \sqrt{\gamma/(2\pi D)}\,\exp[-\gamma x^2/(2D)] \tag{5.29}$$

in agreement with (5.13). For $\gamma \leqq 0$ no stationary solution exists.

The Ornstein-Uhlenbeck process may equally well be described by a linear Langevin equation of the type (3.1) with Gaussian Langevin forces. The stochastic variable and the Langevin force are then connected by the linear transformation (3.7). Because for a linear transformation of variables Gaussian distributions will remain Gaussian (see the remark at the end of Sect. 2.3.3), the transition probability must also be a Gaussian distribution.

Joint Probability Density

In the stationary state the joint probability density for the variables $\xi(t)$ and $\xi(t')$ may be expressed by P and W_{st}. For $t \geqq t'$

$$W_2(x,t;x',t') = P(x,t\,|x',t')\,W_{\mathrm{st}}(x')\,, \tag{5.30}$$

and for $t \leqq t'$,

$$W_2(x,t;x',t') = P(x',t'\,|x,t)\,W_{\mathrm{st}}(x)\,. \tag{5.31}$$

By inserting (5.28, 29) in (5.30, 31) we obtain in both cases

$$W_2(x,t;x',t') = \frac{\gamma}{2\pi D\sqrt{1-\mathrm{e}^{-2\gamma|t-t'|}}}\exp\left(-\gamma\frac{x^2+x'^2-2xx'\,\mathrm{e}^{-\gamma|t-t'|}}{2D(1-\mathrm{e}^{-2\gamma|t-t'|})}\right). \tag{5.32}$$

For large time differences $\gamma|t-t'| \gg 1$, (5.32) decomposes into a product of two stationary distribution functions (5.29), meaning that the distributions for x and x' become independent.

5.4 Eigenfunction Expansion

In this chapter we are looking for nonstationary solutions of (5.1, 2). A separation ansatz for $W(x,t)$

$$W(x,t) = \varphi(x)\mathrm{e}^{-\lambda t} \tag{5.33}$$

leads to

$$L_{\mathrm{FP}}\varphi = -\lambda\varphi\,. \tag{5.34}$$

Here $\varphi(x)$ and λ are the eigenfunctions and eigenvalues of the Fokker-Planck operator with appropriate boundary conditions. Before we proceed it is necessary to talk about boundary conditions.

Boundary Conditions

If the potential $\Phi(x)$ (e.g., $f(x)$ for x-independent diffusion) jumps to an infinite high positive value, the particles cannot penetrate in the region $x > x_{max}$ and therefore the probability current S must vanish at that point. The infinite high potential then acts as a reflecting wall (Fig. 5.1 a). If the potential jumps to an infinite large negative value it follows from the continuity condition for the probability current that $e^{\Phi} W$ should vanish at this point (5.84). In this case we talk about an absorbing wall (Fig. 5.1 b). For the left boundary at $x = x_{min}$ similar considerations are valid. Because of the two possibilities at each side, there are four possibilities B1 ... B4, as shown in Table 5.1.

For finite x_{max} and x_{min}, $e^{\Phi} W = 0$ requires that W should be zero. If $\Phi(x)$ goes to plus infinity for $x \to \pm\infty$ (e.g., $\Phi = \alpha x^2$), we have a reflecting wall at $x_{max} \to +\infty$ and $x_{min} \to -\infty$ and the probability current should vanish there. It then follows from the Fokker-Planck equation that $\int_{-\infty}^{\infty} W(x,t)\mathrm{d}x$ is constant (4.48), and that this constant is equal to 1, if it is initially equal to 1. This normalization requires that the distribution function W goes to zero for $x \to \pm\infty$. (As seen for the parabolic potential in Sect. 5.5.1 $e^{\Phi} W$, however, remains finite.) This boundary condition is called natural boundary condition. It may also happen that $\Phi(x)$ goes to minus infinity for $x \to +\infty$ or for $x \to -\infty$ or for both $x \to \pm\infty$. In this case we require in analogy to (5.84) that $e^{\Phi} W$ is zero at $x \to +\infty$ or at $x \to -\infty$ or at both $x \to \pm\infty$, respectively. As shown in Sect. 5.5.2 for the inverted parabolic potential, W and S are then finite but $e^{\Phi} W$ vanishes at $x \to \pm\infty$. Thus for the boundary condition in Table 5.1 x_{min}, x_{max} or both can reach $-\infty$, $+\infty$ or $\pm\infty$, respectively.

To obtain eigenvalues by numerical integration for potentials, where $\Phi(x)$ goes to plus infinity for $x \to \pm\infty$, we may require that $S = 0$ at $x = \pm A$ for some large A. Alternatively, we may require that $W = 0$ at $x = \pm A$. Though at finite A the eigenvalues for the $S = 0$ condition will be different from the eigenvalues of the $W = 0$ condition, both eigenvalues will coincide in the limit $A \to \infty$. (Obviously, we cannot require that both S and W are zero at $x = \pm A$ with finite A.)

Besides these boundary conditions we may have periodic boundary conditions with period L. If, for instance, x is an angle variable and if we do not distinguish whether a full rotation is made or not, the distribution function and therefore also the probability current must be periodic with period $L = 2\pi$. These periodic boundary conditions can be fulfilled only if the drift and diffusion coefficients are also periodic with the period L. An example of this boundary condition is given in Sect. 11.3.

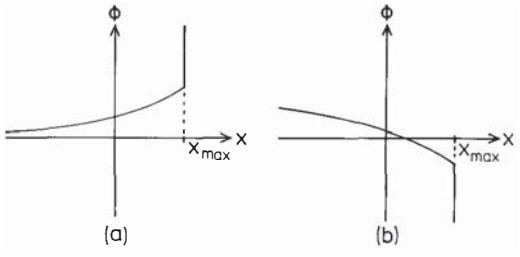

Fig. 5.1. Reflecting **(a)** and absorbing **(b)** wall

Table 5.1. Boundary conditions discussed in the text

x_{min} \ x_{max}	$S = 0$ (reflecting wall)	$e^{\Phi} W = 0$ (absorbing wall)
$S = 0$ (reflecting wall)	B1	B2
$e^{\Phi} W = 0$ (absorbing wall)	B3	B4

Natural boundary conditions:
$S = 0$ for $x_{min} \to -\infty$, $x_{max} \to +\infty$
(i.e. B1 for $x_{min} \to -\infty$, $x_{max} \to +\infty$)

Periodic boundary conditions:
$W(x,t) = W(x+L,t)$, $S(x,t) = S(x+L,t)$

A stationary solution can occur only for the boundary condition B1 (this includes natural boundary conditions) or for periodic boundary conditions. In the first case, the stationary solution of the Fokker-Planck equation is given by (5.13), for the other, by (5.16).

Transformation of the Fokker-Planck Operator

The Fokker-Planck operator (5.2), which may be written in the form, cf. (5.1, 15),

$$L_{FP} = \frac{\partial}{\partial x} D^{(2)}(x) e^{-\Phi(x)} \frac{\partial}{\partial x} e^{\Phi(x)}, \tag{5.35}$$

is obviously not a Hermitian operator. If the two functions W_1 and W_2 both satisfy the same boundary conditions listed in Table 5.1, we have

$$\begin{aligned}
&\int_{x_{min}}^{x_{max}} W_1 e^{\Phi} L_{FP} W_2 \mathrm{d}x \\
&= \int_{x_{min}}^{x_{max}} W_1 e^{\Phi} \frac{\partial}{\partial x} D^{(2)} e^{-\Phi} \frac{\partial}{\partial x} e^{\Phi} W_2 \mathrm{d}x \\
&= -\int_{x_{min}}^{x_{max}} \left[\frac{\partial}{\partial x} W_1 e^{\Phi}\right] D^{(2)} e^{-\Phi} \left[\frac{\partial}{\partial x} e^{\Phi} W_2\right] \mathrm{d}x \\
&= \int_{x_{min}}^{x_{max}} W_2 e^{\Phi} \frac{\partial}{\partial x} D^{(2)} e^{-\Phi} \frac{\partial}{\partial x} W_1 e^{\Phi} \mathrm{d}x \\
&= \int_{x_{min}}^{x_{max}} W_2 e^{\Phi} L_{FP} W_1 \mathrm{d}x .
\end{aligned} \tag{5.36}$$

In deriving the third and the fourth line we have used partial integration and

$$W_1 \mathrm{e}^{\Phi} D^{(2)} \mathrm{e}^{-\Phi} \frac{\partial}{\partial x} \mathrm{e}^{\Phi} W_2 \Big|_{x_{\min}}^{x_{\max}} = -\underset{2}{W_1} \mathrm{e}^{\Phi} \underset{1}{S_2} \Big|_{x_{\min}}^{x_{\max}} = 0 . \tag{5.37}$$

Hence for all boundary conditions of Table 5.1 the adjoint of the operator $\mathrm{e}^{\Phi} \boldsymbol{L}_{\mathrm{FP}}$ is given by

$$(\mathrm{e}^{\Phi} \boldsymbol{L}_{\mathrm{FP}})^{+} \equiv \boldsymbol{L}_{\mathrm{FP}}^{+} \mathrm{e}^{\Phi} = \mathrm{e}^{\Phi} \boldsymbol{L}_{\mathrm{FP}} , \tag{5.38}$$

i.e., $\mathrm{e}^{\Phi} \boldsymbol{L}_{\mathrm{FP}}$ as well as

$$\boldsymbol{L} = \mathrm{e}^{-\Phi/2} \mathrm{e}^{\Phi} \boldsymbol{L}_{\mathrm{FP}} \mathrm{e}^{-\Phi/2} = \mathrm{e}^{\Phi/2} \boldsymbol{L}_{\mathrm{FP}} \mathrm{e}^{-\Phi/2} \tag{5.39}$$

is an Hermitian operator.

Orthogonality of Eigenfunctions

The eigenvalues may be discrete or continuous or both. In the following we use the notation for discrete eigenvalues denoted by an index n. If continuous eigenvalues occur, one should proceed in the same way as discussed in quantum mechanics [5.3], i.e., the Kronecker symbol δ_{nm} has to be replaced by the δ function and the occurring sums by integrations. If $\varphi_n(x)$ are the eigenfunctions of the Fokker-Planck operator $\boldsymbol{L}_{\mathrm{FP}}$ with the eigenvalue λ_n (5.34), the functions

$$\psi_n(x) = \mathrm{e}^{\Phi(x)/2} \varphi_n(x) \tag{5.40}$$

are eigenfunctions of $\boldsymbol{L}$ with the same eigenvalues λ_n

$$\boldsymbol{L} \psi_n = -\lambda_n \psi_n . \tag{5.41}$$

Because $\boldsymbol{L}$ is an Hermitian operator, the eigenvalues are real and two eigenfunctions ψ_1 and ψ_2 with different eigenvalues $\lambda_1 \neq \lambda_2$ must be orthogonal. If we normalize the eigenfunctions we thus have the orthonormality relation

$$\int_{x_{\min}}^{x_{\max}} \psi_n \psi_m \mathrm{d}x = \int_{x_{\min}}^{x_{\max}} \mathrm{e}^{\Phi} \varphi_n \varphi_m \mathrm{d}x = \delta_{nm} . \tag{5.42}$$

Positivity of Eigenvalues

By using the first and the third line of (5.36) with $W_1 = W_2 = \varphi_n(x)$ and (5.35) we get

$$\int_{x_{\min}}^{x_{\max}} \varphi_n \mathrm{e}^{\Phi} \boldsymbol{L}_{\mathrm{FP}} \varphi_n \mathrm{d}x = \int_{x_{\min}}^{x_{\max}} \psi_n \boldsymbol{L} \psi_n \mathrm{d}x = -\lambda_n$$

$$= -\int_{x_{\min}}^{x_{\max}} \left(\frac{\partial}{\partial x} \psi_n \mathrm{e}^{\Phi/2} \right)^2 D^{(2)} \mathrm{e}^{-\Phi} \mathrm{d}x \leqq 0 . \tag{5.43}$$

The equals sign in (5.43) is valid only for the stationary solution

$$\psi_0(x) = \sqrt{N} \mathrm{e}^{-\Phi(x)/2} ; \quad \lambda_0 = 0 . \tag{5.44}$$

All other eigenvalues λ_n ($n \geqq 1$) must be larger than zero. For finite potentials $\Phi(x)$ a stationary solution cannot exist for the boundary conditions B2 – B4. Thus all eigenvalues are larger than zero for these boundary conditions. For (5.44) to exist under natural boundary conditions, $\Phi(x)$ must be positive and increase with increasing $|x|$ at least asymptotically.

Other eigenfunctions with $\lambda_n > 0$ can exist for asymptotically negative $\Phi(x)$, with appropriate boundary conditions, see the example in Sect. 5.5.2.

Completeness Relations

Eigenfunctions of Hermitian operators usually form a complete set [5.1, 2, 4]. The completeness relation for the eigenfunctions ψ_n or φ_n may be expressed by

$$\begin{aligned} \delta(x-x') &= \sum_n \psi_n(x) \psi_n(x') \\ &= \mathrm{e}^{\Phi(x)/2 + \Phi(x')/2} \sum_n \varphi_n(x) \varphi_n(x') \\ &= \mathrm{e}^{\Phi(x)} \sum_n \varphi_n(x) \varphi_n(x') \\ &= \mathrm{e}^{\Phi(x')} \sum_n \varphi_n(x) \varphi_n(x') . \end{aligned} \tag{5.45}$$

Transition Probability Density

By using the last expression of (5.45) to represent the δ function and the formal solution (4.17) for the Fokker-Planck operator, we immediately obtain the expansion of the transition probability into eigenfunctions ($t \geqq t'$)

$$\begin{aligned} P(x,t|x',t') &= \mathrm{e}^{\boldsymbol{L}_{\mathrm{FP}}(x)(t-t')} \delta(x-x') \\ &= \mathrm{e}^{\Phi(x')} \sum_n \mathrm{e}^{\boldsymbol{L}_{\mathrm{FP}}(x)(t-t')} \varphi_n(x) \varphi_n(x') \\ &= \mathrm{e}^{\Phi(x')} \sum_n \varphi_n(x) \varphi_n(x') \mathrm{e}^{-\lambda_n(t-t')} \\ &= \mathrm{e}^{\Phi(x')/2 - \Phi(x)/2} \sum_n \psi_n(x) \psi_n(x') \mathrm{e}^{-\lambda_n(t-t')} . \end{aligned} \tag{5.46}$$

Joint Probability Density

In the stationary state the joint probability density for the variables $\xi(t)$ and $\xi(t')$ may be obtained from (5.30, 31). If the stationary distribution $W_{st}(x) = [\psi_0(x)]^2$ exists, we have

$$W_2(x,t;x',t') = \psi_0(x)\,\psi_0(x') \sum_n \psi_n(x)\,\psi_n(x')\,e^{-\lambda_n|t-t'|}\,. \tag{5.47}$$

The symmetry of W_2, i.e., $W_2(x,t;x',t') = W_2(x',t';x,t)$, is immediately seen.

Explicit Form of L

Because of (5.35) the transformed operator (5.39) takes the form

$$L = e^{\Phi/2}\frac{\partial}{\partial x}\sqrt{D^{(2)}}e^{-\Phi/2}\sqrt{D^{(2)}}e^{-\Phi/2}\frac{\partial}{\partial x}e^{\Phi/2} = -\hat{a}a\,, \tag{5.48}$$

where a and $\hat{a}$ are defined by

$$\begin{aligned} a &= \sqrt{D^{(2)}}e^{-\Phi/2}\frac{\partial}{\partial x}e^{\Phi/2} \\ &= \sqrt{D^{(2)}}\frac{\partial}{\partial x} + \frac{1}{2}\left(\frac{dD^{(2)}}{dx} - D^{(1)}\right)\Big/\sqrt{D^{(2)}}\,, \end{aligned} \tag{5.49}$$

$$\begin{aligned} \hat{a} &= -e^{\Phi/2}\frac{\partial}{\partial x}\sqrt{D^{(2)}}e^{-\Phi/2} \\ &= -\frac{\partial}{\partial x}\sqrt{D^{(2)}} + \frac{1}{2}\left(\frac{dD^{(2)}}{dx} - D^{(1)}\right)\Big/\sqrt{D^{(2)}}\,. \end{aligned} \tag{5.50}$$

The second lines follow by use of (5.14).

For natural boundary conditions a and $\hat{a}$ are the adjoints of each other, i.e., $\hat{a} = a^+$. It then also follows from (5.48) that all eigenvalues λ must be non-negative. By inserting the last expressions for a and $\hat{a}$ into (5.48) we get the operator of the Sturm-Liouville equation [5.1, 2, 4]

$$L = \frac{\partial}{\partial x}D^{(2)}\frac{\partial}{\partial x} - V\,, \tag{5.51}$$

$$V(x) = \frac{1}{4}\left(\frac{dD^{(2)}}{dx} - D^{(1)}\right)^2/D^{(2)} + \frac{1}{2}\frac{dD^{(1)}}{dx} - \frac{1}{2}\frac{d^2D^{(2)}}{dx^2}\,. \tag{5.52}$$

The eigenvalues are usually arranged in increasing order

$$0 \leqq \lambda_0 < \lambda_1 < \lambda_2 < \ldots\,. \tag{5.53}$$

The first eigenfunction ψ_0 has no zeros, the next eigenfunction ψ_1 has one zero and so on [5.2]. If a stationary solution exists the first eigenvalue λ_0 is zero; otherwise it is larger than zero. Whereas a degeneracy cannot occur for the boundary conditions B1 – B4, it can occur for periodic boundary conditions, see Sect. 11.3.2 for an example.

Transformation to a Schrödinger Equation

By using a proper transformation of the variable, the one-variable Fokker-Planck equation can always be transformed to (5.10) where the diffusion constant is x-independent. Then L has the same form as the negative single-particle Hamilton operator in quantum mechanics, i.e.,

$$L = D\frac{\partial^2}{\partial x^2} - V_S(x) \tag{5.54}$$

with the potential

$$V_S(x) = \tfrac{1}{4}[f'(x)]^2/D - \tfrac{1}{2}f''(x)\,. \tag{5.55}$$

For the potential $\Phi(x)$ we may now use

$$\Phi(x) = f(x)/D \tag{5.56}$$

because we can neglect the additive constant $\ln D$ (5.14). The form (5.55) guarantees that the eigenvalue of the stationary solution $\psi_0 = \sqrt{N}\exp[-f(x)/(2D)]$ is zero. The eigenvalue problem (5.41) is the same as the eigenvalue problem of the Schrödinger equation. The operators a and $\hat{a}$ simplify to

$$\begin{aligned} a &= \sqrt{D}\frac{\partial}{\partial x} + \frac{1}{2}\frac{f'(x)}{\sqrt{D}} = \sqrt{D}\exp\left(-\frac{1}{2}\frac{f(x)}{D}\right)\frac{\partial}{\partial x}\exp\left(\frac{1}{2}\frac{f(x)}{D}\right) \\ \hat{a} &= -\sqrt{D}\frac{\partial}{\partial x} + \frac{1}{2}\frac{f'(x)}{\sqrt{D}} = -\sqrt{D}\exp\left(\frac{1}{2}\frac{f(x)}{D}\right)\frac{\partial}{\partial x}\exp\left(-\frac{1}{2}\frac{f(x)}{D}\right) \end{aligned} \tag{5.57}$$

and their commutator is given by

$$a\hat{a} - \hat{a}a = f''\,. \tag{5.58}$$

If the transformation (5.40) is applied to the probability density $W(x,t)$, the Fokker-Planck equation (5.10) is formally equivalent to the time-dependent

Schrödinger equation with imaginary times $t_{\text{Schröd}} = -\mathrm{i}\hbar t$ and with a mass given by $m_{\text{Schröd}} = \hbar^2/(2D)$. Transformation of an equation of the type (5.1, 2) to the Schrödinger form is also found in [5.2, 4].

5.5 Examples

We now want to discuss the eigenvalues, eigenfunctions, the potential $f(x)$ and the potential $V_S(x)$ of the corresponding Schrödinger equation for some examples. We first notice that every soluble example of the Schrödinger equation may serve as a soluble example of the normalized Fokker-Planck equation (5.10) [5.5–9]. From (5.44, 56) the potential $f(x)$ of the normalized Fokker-Planck equation is then expressed by the lowest eigenfunction $\psi_0(x)$ of the Schrödinger equation

$$\begin{aligned} f(x) &= -2D\ln\psi_0(x) + D\ln N \\ f'(x) &= -2D\,\psi_0'(x)/\psi_0(x)\,. \end{aligned} \tag{5.59}$$

Here we have assumed that the stationary solution exists, i.e., that the eigenvalue λ_0 is zero. As will be seen from the third example, simple forms of the potential $V_S(x)$ of the Schrödinger equation may lead to complicated forms of the potential $f(x)$ of the Fokker-Planck equation. This is also seen in [5.6, 7] where simple bistable models for $V_S(x)$ (potential box with a square barrier in the middle) lead to more complicated expressions for $f(x)$. In Sect. 5.7 it is shown that for simple expressions of $f(x)$ (i.e., a box with a rectangular barrier in the middle) eigenvalues and eigenfunctions can also be obtained.

5.5.1 Parabolic Potential

For the parabolic potential of the Fokker-Planck equation

$$f(x) = \tfrac{1}{2}\gamma x^2\,; \qquad \gamma > 0 \tag{5.60}$$

the potential (5.55) of the Schrödinger equation is also parabolic

$$V_S(x) = \gamma\left(\frac{\gamma}{4D}x^2 - \frac{1}{2}\right). \tag{5.61}$$

Introducing the boson operators similar to a and $\hat{a}$ in (5.57)

$$b = \frac{a}{\sqrt{\gamma}} = \frac{1}{\sqrt{2}}\left(\frac{\partial}{\partial\xi} + \xi\right); \qquad \xi = \sqrt{\frac{\gamma}{2D}}\,x$$

$$b^+ = \frac{\hat{a}}{\sqrt{\gamma}} = \frac{1}{\sqrt{2}}\left(-\frac{\partial}{\partial\xi} + \xi\right); \qquad bb^+ - b^+b = 1\,, \tag{5.62}$$

the transformed Fokker-Planck operator (5.48) takes the form

$$L = -\gamma b^+ b\,. \tag{5.63}$$

Eigenvalues and normalized eigenfunctions are given by the well-known expressions [5.3]

$$\begin{aligned} \lambda_n &= \gamma n\,; \qquad n = 0, 1, 2, \ldots \\ \psi_0(x) &= \sqrt[4]{\frac{\gamma}{2\pi D}}\,\mathrm{e}^{-\xi^2/2} \\ \psi_n(x) &= \frac{(b^+)^n}{\sqrt{n!}}\,\psi_0(x) = \sqrt[4]{\frac{\gamma}{2\pi D}}\,\frac{1}{\sqrt{2^n n!}}\,\mathrm{H}_n(\xi)\,\mathrm{e}^{-\xi^2/2}\,, \end{aligned} \tag{5.64}$$

where $\mathrm{H}_n(x)$ are the Hermite polynomials.

If we apply the following summation formula for the Hermite polynomials ([5.10]; $|\alpha| < \frac{1}{2}$)

$$\sum_{n=0}^{\infty}\frac{\alpha^n}{n!}\mathrm{H}_n(x)\mathrm{H}_n(y) = \frac{1}{\sqrt{1-4\alpha^2}}\exp\left[\frac{4\alpha}{1-4\alpha^2}(xy - \alpha x^2 - \alpha y^2)\right], \tag{5.65}$$

we recover from (5.46) the transition probability (5.28) and from (5.47) the joint distribution (5.32) for the Ornstein-Uhlenbeck process.

5.5.2 Inverted Parabolic Potential

For the inverted parabolic potential

$$\bar{f}(x) = -\tfrac{1}{2}\bar{\gamma}x^2\,; \qquad \bar{\gamma} > 0 \tag{5.66}$$

no stationary solution exists. Nevertheless we can make the transformation (5.39, 40) with $\Phi(x) = \bar{f}(x)/D = -\frac{1}{2}\bar{\gamma}x^2/D$ and obtain the following potential $\bar{V}_S(x)$ of the Schrödinger equation:

$$\bar{V}_S(x) = \bar{\gamma}\left(\frac{\bar{\gamma}}{4D}x^2 - \frac{1}{2}\right) + \bar{\gamma}\,. \tag{5.67}$$

A comparison with (5.61) shows that the normalized eigenfunctions are the same as in Sect. 5.5.1 with γ replaced by $\bar{\gamma}$, i.e.,

$$\bar{\psi}_n(x) = \sqrt[4]{\frac{\bar{\gamma}}{2D\pi}} \frac{1}{\sqrt{2^n n!}} H_n(\bar{\xi}) e^{-\bar{\xi}^2/2}; \quad \bar{\xi} = \sqrt{\frac{\bar{\gamma}}{2D}} x \tag{5.68}$$

and that the eigenvalues are raised by $\bar{\gamma}$, i.e., they start with $\lambda_0 = \bar{\gamma}$

$$\bar{\lambda}_n = \bar{\gamma}(n+1); \quad n = 0, 1, 2, \ldots . \tag{5.69}$$

(By formally changing γ to $\bar{\gamma}$ in (5.62) and ξ in $i\bar{\xi}$ it is seen that $-a/\sqrt{\bar{\gamma}}$ now becomes a creation operator b^+ and correspondingly that $-\hat{a}/\sqrt{\bar{\gamma}}$ now becomes an annihilation operator b, cf. Sect. 5.8.)

Using both (5.46, 65) we obtain

$$P(x,t|x',t') = \sqrt{\frac{\bar{\gamma}}{2\pi D(1-e^{-2\bar{\gamma}(t-t')})}} \exp\left(-\frac{\bar{\gamma}(x e^{-\bar{\gamma}(t-t')} - x')^2}{2D(1-e^{-2\bar{\gamma}(t-t')})}\right) e^{-\bar{\gamma}(t-t')}, \tag{5.70}$$

which is identical to (5.28) if γ in (5.28) is replaced by $-\bar{\gamma}$. Though no stationary solution exists for an inverted parabolic potential, eigenfunctions with the boundary condition B4 in Table 5.1. for $x_{\substack{\max \\ \min}} \to \pm\infty$ do exist, they can be normalized according to (5.42) and they may be used to calculate the transition probability. (The probability current S for these eigenfunctions is finite for $x \to \pm\infty$.)

5.5.3 Infinite Square Well for the Schrödinger Potential

One of the simplest eigenvalue problems for the Schrödinger equation is the rectangular-well potential with infinitely high walls, Fig. 5.2. The lowest eigenfunction $\psi_0(x) = a^{-1/2}\cos[\pi x/(2a)]$ for $-a < x < a$ leads to the potential (5.59)

$$f(x) = -2D\ln\{\cos[\pi x/(2a)]\} \tag{5.71}$$

of the Fokker-Planck equation, plotted in Fig. 5.2. [In (5.71) we have normalized the potential by $f(0) = 0$, i.e., $N = a^{-1}$.] At $x = \pm a$ the potential $f(x)$ becomes singular. It may easily be checked that the probability density as well as the probability current are zero at $x = \pm a$. Higher eigenvalues and normalized eigenfunctions of the transformed Fokker-Planck operator (5.54) are

even solutions ($n = 1, 2, \ldots$)

$$\lambda_{2n} = D\pi^2 a^{-2}(n^2+n), \tag{5.72}$$

$$\psi_{2n}(x) = a^{-1/2}\cos[(n+1/2)\pi x/a], \tag{5.73}$$

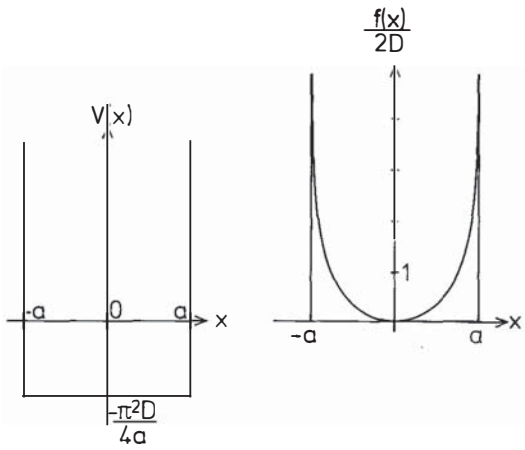

Fig. 5.2. Rectangular-well potential $V(x)$ and the corresponding potential $f(x)$ of the Fokker-Planck equation, (5.71)

odd solutions ($n = 1, 2, \ldots$)

$$\lambda_{2n-1} = D\pi^2 a^{-2}(n^2 - 1/4), \tag{5.74}$$

$$\psi_{2n-1}(x) = a^{-1/2}\sin(n\pi x/a). \tag{5.75}$$

The transition probability for the potential (5.71) is obtained by inserting (5.72 – 75) into (5.46).

5.5.4 *V*-shaped Potential for the Fokker-Planck Equation

If the potential of the Fokker-Planck equation is given by the *V*-shaped form

$$f(x) = D\kappa|x|; \quad \kappa > 0, \tag{5.76}$$

the Schrödinger potential $V_S(x)$ consists, see (5.55), of an attractive δ potential

$$V_S(x) = D\kappa^2/4 - D\kappa\delta(x). \tag{5.77}$$

Only the stationary eigenfunction

$$\psi_0(x) = \sqrt{\kappa/2}\, e^{-\kappa|x|/2} \tag{5.78}$$

has the discrete eigenvalue $\lambda_0 = 0$. The other eigenvalues form a continuum ($k > 0$)

$$\lambda_k = D\kappa^2/4 + Dk^2; \tag{5.79}$$

their eigenfunctions normalized to the δ function are [5.11]

$$\psi_k^s(x) = [(4k^2+\kappa^2)\,\pi]^{-1/2}(2k\cos kx - \kappa \sin k|x|)$$
$$\psi_k^a(x) = \pi^{-1/2}\sin kx\,. \tag{5.80}$$

The symbols s and a indicate even or symmetric and odd or antisymmetric eigenfunctions.

The transition probability for the potential (5.76) is obtained from (5.46), where the sum in (5.46) must be replaced by an integration over k for the continuous eigenfunctions while the discrete eigenfunctions must be retained as a single term.

5.6 Jump Conditions

For the Schrödinger equation one often uses potential models where $V_S(x)$ jumps at certain points of x and is constant elsewhere. One may ask whether such models may also be used for the potential $f(x)$ of the Fokker-Planck equation. As is seen from (5.55), jumps of the potential $f(x)$ lead to higher singularities (first derivative of the δ function and square of the δ function) for the potential $V_S(x)$ than δ function singularities which are usually treated in quantum mechanics. We first derive the jump conditions for the unnormalized Fokker-Planck equation (5.1, 2) and then specialize the result to the normalized Fokker-Planck equation (5.10).

Finite Jump

We assume that a finite jump of the potential $\Phi(x)$ (5.14) occurs at $x=0$. A finite jump may occur either if the diffusion coefficient $D^{(2)}(x)$ has a finite jump or if the drift coefficient $D^{(1)}(x)$ has a δ function singularity. If we assume that the time derivative of the probability density is finite at the jump, it follows from the continuity equation (4.46) that the probability current (5.15) must be continuous ($\partial/\partial x$ is denoted by a prime)

$$\begin{aligned} S(+0,t) &= -D^{(2)}(+0)[\Phi'(+0)\,W(+0,t) + W'(+0,t)] \\ &= S(-0,t) = -D^{(2)}(-0)[\Phi'(-0)\,W(-0,t) + W'(-0,t)]\,. \end{aligned} \tag{5.81}$$

Here $\lim_{\varepsilon\to 0} f(\pm|\varepsilon|)$ was abbreviated by $f(\pm 0)$. (If the probability current would not be continuous at $x=0$ this would mean that at $x=0$ particles are added or removed, i.e. that we have a probability source or sink at $x=0$.) Furthermore it follows from (5.15) that we may write

$$\frac{\partial}{\partial x}[e^{\Phi(x)}W(x,t)] = -S(x,t)e^{\Phi(x)}/D^{(2)}(x)\,.$$

By formally integrating this expression we get

$$e^{\Phi(+0)}W(+0,t) - e^{\Phi(-0)}W(-0,t) = -\lim_{\varepsilon\to 0}\int_{-\varepsilon}^{\varepsilon} S(x,t)e^{\Phi(x)}/D^{(2)}(x)\,dx\,.$$

If only finite jumps in $\Phi(x)$ and $D^{(2)}(x) > 0$ occur, the integral vanishes for $\varepsilon \to 0$, i.e., we have

$$e^{\Phi(+0)}W(+0,t) = e^{\Phi(-0)}W(-0,t)\,. \tag{5.82}$$

Equations (5.81, 82) are the jump conditions for the probability density.

Infinite Jumps

If the integral in (5.14) is finite for $x \leqq x_{max}$ but has an infinite positive value for $x > x_{max}$ no diffusion into the region $x > x_{max}$ can occur. Therefore the probability current (5.15) must be zero for $x = x_{max}$, i.e.,

$$\Phi'(x_{max})\,W(x_{max},t) = -W'(x_{max},t)\,. \tag{5.83}$$

If the integral in (5.14) is finite for $x \leqq x_{max}$ but has an infinite negative value for $x > x_{max}$ and if we assume that $W(x,t)$ is finite for $x > x_{max}$ it follows from the jump condition (5.82) that $\exp(\Phi)\,W$ must be zero for $x \to x_{max}$, i.e.

$$\exp[\Phi(x_{max}-0)]\,W(x_{max}-0,t) = 0\,.$$

For finite $\Phi(x_{max}-0)$ this reduces to the condition that the probability distribution itself must be zero for $x \to x_{max}$,

$$W(x_{max}-0,t) = 0\,. \tag{5.84}$$

Similar results are valid if the jump occurs at x_{min}.

Jump Conditions for the Eigenfunctions

For the normalized equation (5.10) the jump conditions for the eigenfunctions (5.40) of the operator (5.54) corresponding to (5.81 – 84) then take the form [5.12]

$$\begin{aligned} &\exp\left(-\frac{f(+0)}{2D}\right)\left[\psi_n'(+0) + \frac{f'(+0)}{2D}\psi_n(+0)\right] \\ &= \exp\left(-\frac{f(-0)}{2D}\right)\left[\psi_n'(-0) + \frac{f'(-0)}{2D}\psi_n(-0)\right] \end{aligned} \tag{5.81a}$$

$$\exp\left(\frac{f(+0)}{2D}\right)\psi_n(+0) = \exp\left(\frac{f(-0)}{2D}\right)\psi_n(-0)\,, \tag{5.82a}$$

$$2D\,\psi_n'(x_{\max}-0) = -f'(x_{\max}-0)\,\psi_n(x_{\max}-0)\,, \tag{5.83a}$$

$$\psi_n(x_{\max}-0) = 0\,. \tag{5.84a}$$

These jump conditions are valid for any potential with continuous values and derivatives between the jumps. However, if the potential is linear between the jumps, the transformed potential $V_S(x)$ is a constant and the solutions of the differential equation are immediately obtained between the jumps. Each jump condition then leads to one homogeneous equation, the whole set of those equations having only nontrivial solutions if the determinant is zero. This condition is in general a transcendental equation, which determines the eigenvalues and eigenfunctions. For simple potential wells the transcendental equation may be solved analytically, as in the following example.

5.7 A Bistable Model Potential

As an example we treat the following bistable rectangular potential well (Fig. 5.3)

$$\begin{aligned} f(x) &= f_0\,, \quad |x| \leqq L/2 \\ f(x) &= 0\,, \quad L/2 < |x| \leqq L \\ f(x) &= \infty\,, \quad x > L\,. \end{aligned} \tag{5.85}$$

It turns out that for this special bistable model all eigenvalues and eigenfunctions can be obtained analytically. (If the width of the barrier in the middle is not half the total width of the box a transcendental equation has to be solved.)

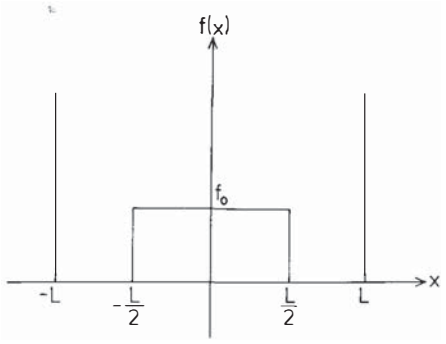

Fig. 5.3. Bistable potential model

With the help of the jump conditions (5.81a–83a) we easily obtain the following eigenvalues and normalized eigenfunctions:

even eigenfunctions and their eigenvalues

$$\lambda_{4n} = (\pi^2 D/L^2)(2n)^2\,; \qquad (n = 0, 1, 2, \ldots) \tag{5.86}$$

$$\psi_0 = [L(1+\mathrm{e}^{-f_0/D})]^{-1/2}\mathrm{e}^{-f(x)/(2D)}\,, \tag{5.87}$$

$$\psi_{4n} = \sqrt{2}[L(1+\mathrm{e}^{-f_0/D})]^{-1/2}\mathrm{e}^{-f(x)/(2D)}\cos 2n\pi x/L\,; \quad (n = 1, 2, 3, \ldots)\,, \tag{5.88}$$

$$\lambda_{4n+2} = (\pi^2 D/L^2)(2n+1)^2\,; \qquad (n = 0, 1, 2, \ldots)\,, \tag{5.89}$$

$$\psi_{4n+2} = \sqrt{2}[L(1+\mathrm{e}^{f_0/D})]^{-1/2}\mathrm{e}^{f(x)/(2D)}\cos(2n+1)\pi x/L\,, \tag{5.90}$$

odd eigenfunctions and their eigenvalues

$$\lambda_{4n+1} = (\pi^2 D/L^2)(2n+\nu)^2\,; \quad n = 0, 1, 2, \ldots\,, \tag{5.91}$$

$$\begin{aligned} \psi_{4n+1} &= L^{-1/2}\sin[(2n+\nu)x\pi/L]\,; \quad 0 \leqq x < L/2 \\ \psi_{4n+1} &= L^{-1/2}\cos[(2n+\nu)(L-x)\pi/L]\,; \quad L/2 < x < L \end{aligned} \tag{5.92}$$

$$\lambda_{4n-1} = (\pi^2 D/L^2)(2n-\nu)^2\,; \quad n = 1, 2, 3, \ldots\,, \tag{5.93}$$

$$\begin{aligned} \psi_{4n-1} &= L^{-1/2}\sin[(2n-\nu)x\pi/L]\,; \quad 0 \leqq x < L/2 \\ \psi_{4n-1} &= L^{-1/2}\cos[(2n-\nu)(L-x)\pi/L]\,; \quad L/2 < x < L\,. \end{aligned} \tag{5.94}$$

Here ν is defined by

$$\nu = (2/\pi)\arctan\{\exp[-f_0/(2D)]\}\,; 0 < \nu < 1\,. \tag{5.95}$$

Some of the lowest eigenvalues and their eigenfunctions are shown in Figs. 5.4, 5. In particular, the lowest nonzero eigenvalue reads

$$\lambda_1 = (4D/L^2)[\arctan\{\exp[-f_0/(2D)]\}]^2\,, \tag{5.96}$$

which in the limit of large barrier heights is proportional to the Boltzmann factor, i.e.,

$$\lambda_1 = (4D/L^2)\exp(-f_0/D) \quad \text{for} \quad f_0/D \gg 1\,. \tag{5.96a}$$

Some other bistable models and a soluble metastable and a periodic potential model are given in [5.12]. The last model is also treated in Sect. 11.3.2. By inverting the potential (5.85) one also gets a metastable model (Sect. 5.8).

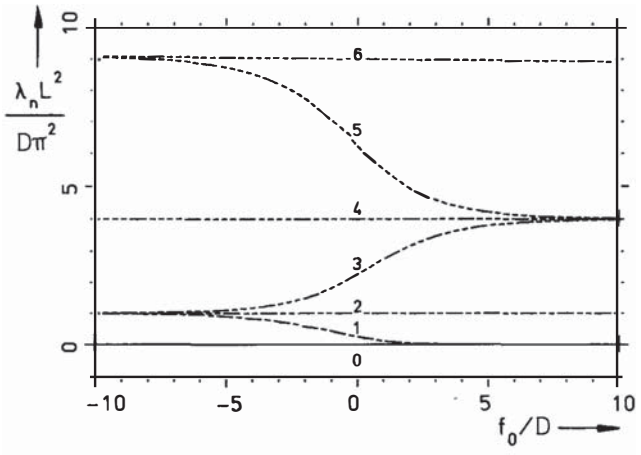

Fig. 5.4. The eigenvalues λ_n, $n = 0, 1, \ldots, 6$ of the bistable rectangular potential well as a function of f_0/D

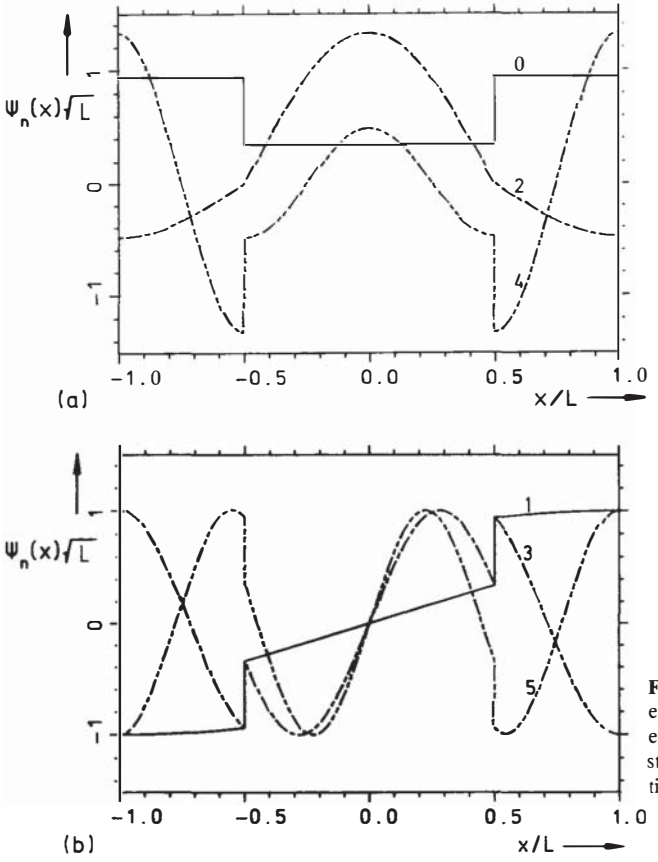

Fig. 5.5. The first three even **(a)** and odd **(b)** eigenfunctions of the bistable rectangular potential well for $f_0 = 2D$

5.8 Eigenfunctions and Eigenvalues of Inverted Potentials

In addition to the normalized Fokker-Planck equation (5.10) we consider this equation for the inverted (upside-down) potential

$$\bar{f}(x) = -f(x)\,, \tag{5.97}$$

but with the same x-independent diffusion constant D. As easily seen from (5.57), the operators $\bar{a}$ and $\hat{\bar{a}}$ for the inverted potential are connected with the operators a and $\hat{a}$ by the simple relations

$$\bar{a} = -\hat{a}\,; \quad \hat{\bar{a}} = -a\,. \tag{5.98}$$

Therefore the operator (5.48) for the inverted potential may be written as

$$\bar{L} = -\hat{\bar{a}}\bar{a} = -a\hat{a}\,. \tag{5.99}$$

We now apply the operator a to the eigenvalue equation $L\psi_n = -\lambda_n\psi_n$, i.e.,

$$aL\psi_n = -a\hat{a}a\psi_n = \bar{L}a\psi_n = -\lambda_n a\psi_n\,. \tag{5.100}$$

Thus if $a\psi_n$ is not identical to zero it is an eigenfunction of the operator belonging to the inverted problem.

The connection between the nth eigenfunction ψ_n of the original problem and the mth eigenfunction ψ_m of the inverted problem depends on the boundary conditions. Therefore we first discuss the transformation of the boundary conditions. Using $\varphi_n(x) = \exp[-(1/2)f(x)/D]\,\psi_n(x)$, $\bar{\varphi}_m(x) = \exp[-(1/2)\bar{f}(x)/D] \cdot \bar{\psi}_m(x)$, (5.57) and $\bar{\psi}_m \sim a\psi_n$ the probability current may be written in the form

$$\begin{aligned} S(x) &= -D\exp\left(-\frac{f(x)}{D}\right)\frac{\partial}{\partial x}\left[\exp\left(\frac{f(x)}{D}\right)\varphi_n(x)\right] \\ &= -D\exp\left(-\frac{f(x)}{2D}\right)\exp\left(-\frac{f(x)}{2D}\right)\frac{\partial}{\partial x}\left[\exp\left(\frac{f(x)}{2D}\right)\psi_n(x)\right] \\ &= -\sqrt{D}\exp\left(-\frac{f(x)}{2D}\right)a\psi_n(x) \\ &\sim \exp\left(-\frac{f(x)}{2D}\right)\bar{\psi}_m(x) = \exp\left(\frac{f(x)}{D}\right)\bar{\varphi}_m(x)\,. \end{aligned}$$

Thus the boundary condition

$$S(x_0) = -D\exp\left(-\frac{f(x_0)}{D}\right)\frac{\partial}{\partial x}\left[\exp\left(\frac{f(x)}{D}\right)\varphi_n(x)\right]\Bigg|_{x=x_0} = 0$$

for $\varphi_n(x)$ is transformed to the boundary condition

$$\exp\left(\frac{\bar{f}(x_0)}{D}\right)\bar{\varphi}_m(x_0)=0$$

for the eigenfunction $\bar{\varphi}_m(x)$. Similarly the boundary condition

$$\exp\left(\frac{f(x_0)}{D}\right)\varphi_n(x_0)=0$$

for $\varphi_n(x)$ is transformed to the boundary condition

$$\bar{S}(x_0)=-D\exp\left(-\frac{\bar{f}(x_0)}{D}\right)\frac{\partial}{\partial x}\left[\exp\left(\frac{\bar{f}(x)}{D}\right)\bar{\varphi}_m(x)\right]\Bigg|_{x=x_0}=0$$

for the eigenfunctions $\bar{\varphi}_m$ of the inverted potential, in agreement with Table 5.1. (By inverting the potential a reflecting wall is transformed to an absorbing wall and vice versa). As may be checked the jump conditions for ψ_n and the jump conditions for $\bar{\psi}_m$ are connected according to

(5.81a)		$\Leftrightarrow$ (5.82a)	
(5.82a)		$\Leftrightarrow$ (5.81a)	
(5.83a)	for ψ_n	$\Leftrightarrow$ (5.84a)	for $\bar{\psi}_m$.
(5.84a)		$\Leftrightarrow$ (5.83a)	

(To see these connections $\psi_n=\bar{a}\bar{\psi}_m/\sqrt{\lambda_m}=-\hat{a}\bar{\psi}_m/\sqrt{\lambda_m}$ may be used; notice that normalized real eigenfunctions are defined only up to a factor ± 1.)

We now express the eigenvalues and normalized eigenfunctions of the operator $\bar{L}$ in terms of those of the operator L. To find the normalized functions

$$\int(a\psi_n)(a\psi_n)\mathrm{d}x=\int\psi_n(\hat{a}a\psi_n)\mathrm{d}x=\lambda_n$$

may be used. According to the various boundary conditions in Table 5.1 we have the following possibilities:

1) Boundary condition B1 (this includes natural boundary conditions) for the original problem, i.e. B4 for the inverted problem ($\lambda_0=0$; $a\psi_n=0$)

$$\bar{\lambda}_n=\lambda_{n+1}>0\,;\qquad \bar{\psi}_n=a\psi_{n+1}/\sqrt{\lambda_{n+1}}\,,\qquad n=0,1,2,\ldots\,. \tag{5.101a}$$

2) Boundary conditions B2 (B3) for the original problem, i.e. B3 (B2) for the inverted problem

$$\bar{\lambda}_n=\lambda_n>0\,;\qquad \bar{\psi}_n=a\psi_n/\sqrt{\lambda_n}\,,\qquad n=0,1,2,\ldots \tag{5.101b}$$

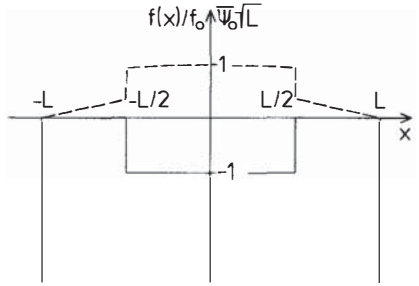

Fig. 5.6. Metastable potential model (*solid line*) and its lowest eigenfunction (*broken line*) for $f_0=2D$

3) Boundary condition B4 for the original problem, i.e. B1 for the inverted problem

$$\bar{\lambda}_0=0\,,\quad \bar{\lambda}_{n+1}=\lambda_n>0\,,\quad \bar{\psi}_{n+1}=a\psi_n/\sqrt{\lambda_n}\,,\quad n=0,1,2,\ldots\,. \tag{5.101c}$$

4) Periodic boundary conditions ($\lambda_0=\bar{\lambda}_0=0$)

$$\bar{\lambda}_n=\lambda_n>0\,,\qquad \bar{\psi}_n=a\psi_n/\sqrt{\lambda_n}\,,\qquad n=1,2,\ldots\,. \tag{5.101d}$$

The eigenfunction $\bar{\psi}_0$ in case 3 and 4 must be obtained from $\bar{a}\bar{\psi}_0=0$. The eigenvalues and eigenfunctions of the operator belonging to the parabolic potential and the inverted parabolic potential (Sects. 5.5.1, 2) are examples of (5.101a, c).

Inverting the bistable potential model in Sect. 5.7 gives a metastable potential model. The lowest eigenvalue of this metastable model is then given by $\bar{\lambda}_0=\lambda_1$ (5.96) and the corresponding even eigenfunction by (Fig. 5.6)

$$\begin{aligned}\bar{\psi}_0&=L^{-1/2}\cos\nu\pi x/L\,, && 0\leqq x<L/2\\ \bar{\psi}_0&=L^{-1/2}\sin\nu(L-x)\,\pi/L\,, && L/2<x\leqq L\,.\end{aligned} \tag{5.92a}$$

Here ν is defined by (5.95).

5.9 Approximate and Numerical Methods for Determining Eigenvalues and Eigenfunctions

Because the Fokker-Planck equation can be transformed to a Schrödinger equation, approximate and numerical methods used for solving the Schrödinger equation can also be used for solving the Fokker-Planck equation. We now want to discuss some of these methods which turn out to be quite effective. The Fokker-Planck equation is equivalent to a certain Langevin equation. The computer-simulation method for Langevin equations was already discussed in Sect. 3.6, therefore it will not be repeated here.

5.9.1 Variational Method

Assuming natural boundary conditions (for other types, see [5.2]) the Sturm-Liouville eigenvalue problem (5.41, 51, 52) is equivalent to the following variational problem. The function ψ which minimizes

$$\lambda = \frac{\int \left[\left(\frac{\partial \psi}{\partial x} \right)^2 D^{(2)}(x) + \psi^2 V_S(x) \right] dx}{\int \psi^2 dx} \tag{5.102}$$

leads to the eigenfunction ψ_0. The minimum of this expression is then the lowest eigenvalue λ_0. The next eigenfunction and eigenvalue are found by minimizing (5.102) subject to the auxiliary condition

$$\int \psi_0 \psi dx = 0 . \tag{5.103}$$

Higher eigenfunctions and eigenvalues are found similarly by adding the auxiliary condition that the function is orthogonal to all previous ones [5.2].

Approximate eigenvalues and eigenfunctions are obtained by the following procedure. One guesses some of the lowest eigenfunctions which in addition depend on certain parameters. One then minimizes (5.102) successively subject to $0, 1, 2, 3, \ldots$ auxiliary conditions. In this way, the parameters are determined, leading to approximate eigenfunctions and eigenvalues. From the practical point of view it is preferable to use such functions for the ansatz of the eigenfunctions so that the integral can be evaluated analytically. As for all variational methods, the results for the eigenvalues are much more accurate than those for the eigenfunctions and they are most effective for determining the lowest eigenvalues.

Lower and Upper Bounds

By the modified Ritz method of *Weinstein* [5.13] (see also [5.14]), one obtains lower and upper bounds for the eigenvalues. *Brand* et al. [5.15] applied this method to some Fokker-Planck equations.

5.9.2 Numerical Integration

Let us discuss the numerical integration method for the operator (5.54) of the Schrödinger equation. The method can also be applied to the Fokker-Planck operator (5.2) or to (5.51).

First assume that the potential (5.55) is symmetric, i.e. $V(x) = V(-x)$. The eigenfunctions ψ_s and ψ_a must then be either symmetric or antisymmetric. For the symmetric (antisymmetric) eigenfunction we start integrating at $x = 0$ with the initial condition $\psi(0) = A$; $\psi'(0) = 0$ ($\psi(0) = 0$, $\psi'(0) = A$) up to the boundary $x = x_B$ for some fixed value of λ. (If natural boundary conditions are considered x_B has to be chosen large enough consistent with the desired accuracy of the eigenvalues.) We then calculate the difference to the given boundary values and, by varying λ, determine the eigenvalues λ_n as the zeros of this difference. The eigenfunctions for λ_n are calculated in the above steps and can be normalized by choosing A suitably.

If the potential $V(x)$ is not symmetric but if x_{min}, x_{max} or both are finite and if no singularities in the differential equation occur, we start at $x = x_{min}$ (or at x_{max}) and integrate (5.41) up to x_{max} (x_{min}) using the boundary condition at $x = x_{min}$ (x_{max}). The eigenvalue λ is determined so that at $x = x_{max}$ (x_{min}) the boundary condition is also fulfilled. If x_{max} (x_{min}) is infinite we have to use an appropriately large $x_{max}^{(ap)}$ ($x_{min}^{(ap)}$). If there are singularities in the differential equation at some point, one should try an analytical power expansion around this point and use numerical integration in the other region.

If the potential $V(x)$ is not symmetric and if $x_{min} = -\infty$ and $x_{max} = \infty$, one may start at $x = 0$ with the initial condition $\psi(0) = A$, $\psi'(0) = B$ and integrate (5.41) in both directions to $-\infty$ and $+\infty$. By a proper choice of B and λ both boundary conditions can be fulfilled. In order to find these values of B and λ a regula falsi method for the two variables may be used. The constant A finally follows from the normalization (5.42). Numerical integration methods are usually very accurate even for higher eigenfunctions. In limiting cases, e.g., very high potentials or very small noise strength D, the numerical integration does not work. In these cases, however, analytical methods may be suitable, Sect. 5.10.

5.9.3 Expansion into a Complete Set

To solve the Fokker-Planck equation (5.1, 2) one may expand the probability density into a complete set $\varphi^q(x)$ satisfying the boundary conditions, i.e.,

$$W(x,t) = F(x) \sum_q c^q(t) \varphi^q(x) . \tag{5.104}$$

The choice of the arbitrary function $F(x)$ will be discussed below. For natural boundary conditions $x_{min} = -\infty$ and $x_{max} = \infty$ one may use for $\varphi^q(x)$ for instance Hermite functions $\sim H_q(\alpha x) \exp(-\alpha^2 x^2/2)$, where α is a suitable scaling factor. Another possible choice for $\varphi^q(x)$ is the following. We may construct a system of polynomials orthogonal to a certain weight function [5.16]. As weight function we may use the stationary solution of the Fokker-Planck equation. With the latter choice one has the advantage that φ^q are adapted to the problem under consideration. If we use Hermite functions, only the scaling factor α can be adapted to the problem. The insertion of (5.104) into the Fokker-Planck equation leads to an infinite system of coupled differential equations for the expansion coefficients c^q. The truncated infinite system may then be solved. Sometimes the structure of the system of coupled differential equations may be such that only a finite number M of nearest-neighbor coefficients is coupled, i.e., of the form (9.17). Then one can cast the system into the form of the tridiagonal vector recurrence relation (9.10 or 121) which may be solved by matrix continued-fraction methods as discussed in Chap. 9. The matrix continued-fraction method has the advantage that a large number of expansion terms in (5.104) can be taken into account.

The M-nearest-neighbor coupling of the system seems at first glance to be valid only for very special Fokker-Planck operators. This is, however, not the case. If the drift and diffusion coefficients are rational functions of x, i.e.,

$$D^{(1)}(x) = \frac{P_1(x)}{P_2(x)} = \frac{a_0^{(1)} + a_1^{(1)}x + \ldots + a_{n_1}^{(1)}x^{n_1}}{a_0^{(2)} + a_1^{(2)}x + \ldots + a_{n_2}^{(2)}x^{n_2}},$$
$$D^{(2)}(x) = \frac{P_3(x)}{P_4(x)} = \frac{a_0^{(3)} + a_1^{(3)}x + \ldots + a_{n_3}^{(3)}x^{n_3}}{a_0^{(4)} + a_1^{(4)}x + \ldots + a_{n_4}^{(4)}x^{n_4}}, \quad (5.105)$$

and if there are natural boundary conditions, one can always find such a system with M-nearest-neighbor coupling by using Hermite functions and setting $F(x)$ equal to the product $P_2(x)P_4(x)$ of the denominators in (5.105). (In (5.105) it is tacitly assumed that the denominators are different from zero.) Generally, the function $F(x)$ should be chosen so that M is as small as possible. In [5.17] this method has been applied to the Fokker-Planck equation of a driven Josephson junction, where the drift coefficient is proportional to $a+x+(b+cx^2)^{-1}$ and the diffusion coefficient is a constant. An application to the laser Fokker-Planck equation, where an expansion into Laguerre functions has been made, will be discussed in Sect. 12.4.

5.10 Diffusion Over a Barrier

We first apply the Fokker-Planck equation (5.10) to calculate escape rates over a potential barrier, closely following the work of *Kramers* [1.17]. Then we want to calculate the lowest nonzero eigenvalue for a bistable potential and the lowest eigenvalue for a metastable potential. These types of problems have been extensively treated in the literature [1.6, 7, 5.18–30]. In this section we are mainly interested in the case where the diffusion coefficient D is small, or more precisely where the barrier height Δf is much larger than the diffusion coefficient D. As it turns out, one can get analytic expressions for the escape rate as well as for the lowest nonzero eigenvalue in a bistable potential in this limiting case. For smaller $\Delta f/D$ ratios, where no analytic expressions are generally available, one has to apply numerical methods, which, as discussed in the last section, work for not too large $\Delta f/D$ ratios.

For very low diffusion constants, the coefficient in front of the second derivative in (5.54) becomes very small. Therefore one may use singular perturbation methods [5.31] which have been applied to a bistable potential by *Larson* and *Kostin* [5.23] and *Dekker* [5.27]. In quantum mechanics, where the same problem occurs when one goes over to the classical limit, one uses the WKB method. This method was applied to a bistable potential by *Caroli* et al. [5.24]. More elaborate methods like the path integral method [5.28] and the Liouville projection operator method [5.29] have also been applied. In this chapter we are interested only in the quasi-stationary process. If one starts with a state where the particles are at the top of the barrier, being unstable, it will decay. The transients of such an unstable state will be discussed in Sect. 12.5 in connection with the transients of a laser model.

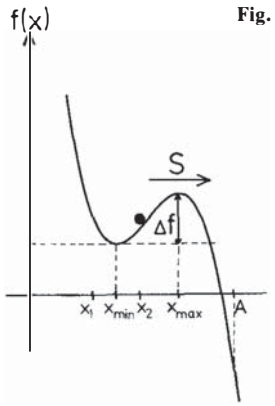

Fig. 5.7. Potential well for calculating the escape rate

5.10.1 Kramers' Escape Rate

We now want to calculate the escape rate for particles sitting in a deep well near $x = x_{\min}$, Fig. 5.7. We assume that $\Delta f/D$ is very large. Furthermore, we restrict ourselves to a constant diffusion D, which, according to Sect. 5.1, can always be achieved by proper transformation. Then the probability current S over the top of the potential barrier near $x_{\max}$ is very small and the time change of the probability density $W(x,t)$ is also very small. For this quasi-stationary state the small probability current S must then be approximately independent of x (4.46). Integrating (5.15) with (5.56), i.e.,

$$-D\,\mathrm{e}^{-f(x)/D}\frac{\partial}{\partial x}\left[\mathrm{e}^{f(x)/D}W(x,t)\right] = S$$

between $x_{\min}$ and A we obtain

$$D\left[\mathrm{e}^{f(x_{\min})/D}W(x_{\min},t) - \mathrm{e}^{f(A)/D}W(A,t)\right] = S\int_{x_{\min}}^{A}\mathrm{e}^{f(x)/D}\mathrm{d}x\,;$$

or if we assume that at $x = A$ the probability density is nearly zero (particles may for instance be taken away) we can express the probability current by the probability density at $x = x_{\min}$, i.e.,

$$S = D\mathrm{e}^{f(x_{\min})/D}W(x_{\min},t)/\int_{x_{\min}}^{A}\mathrm{e}^{f(x)/D}\mathrm{d}x\,. \quad (5.106)$$

If the barrier is high the distribution function near $x_{\min}$ will be given approximately by the stationary distribution

$$W(x,t) = W(x_{\min},t)\,\mathrm{e}^{-[f(x)-f(x_{\min})]/D}\,. \quad (5.107)$$

The probability p to find the particle near $x_{\min}$ reads

$$p = \int_{x_1}^{x_2} W(x,t)\,\mathrm{d}x = W(x_{\min},t)\,\mathrm{e}^{f(x_{\min})/D} \int_{x_1}^{x_2} \mathrm{e}^{-f(x)/D}\mathrm{d}x\,. \tag{5.108}$$

Because for small D the probability density (5.107) becomes very small for x values appreciably different from $x_{\min}$, the x_1, x_2 values need not be specified in detail.

The probability p times the escape rate r is the probability current S. Thus by using (5.106, 108) we get the following expression for the inverse of the escape rate:

$$\frac{1}{r} \equiv \frac{p}{S} = \frac{1}{D} \int_{x_1}^{x_2} \mathrm{e}^{-f(x)/D}\mathrm{d}x \int_{x_{\min}}^{A} \mathrm{e}^{f(x)/D}\mathrm{d}x\,. \tag{5.109}$$

Whereas the main contribution to the first integral stems from the region around $x_{\min}$, the main contribution to the second integral stems from the region around $x_{\max}$. We therefore expand $f(x)$ for the first and second integrals according to

$$\begin{aligned} f(x) &\approx f(x_{\min}) + \tfrac{1}{2} f''(x_{\min})(x - x_{\min})^2 \\ f(x) &\approx f(x_{\max}) - \tfrac{1}{2} |f''(x_{\max})|(x - x_{\max})^2\,. \end{aligned} \tag{5.110}$$

Then we may extend the integration boundaries in both integrals to $\pm\infty$ and thus obtain the well-known Kramers' escape rate

$$r_{\mathrm{K}} = (2\pi)^{-1} \sqrt{f''(x_{\min})\,|f''(x_{\max})|}\,\mathrm{e}^{-[f(x_{\max}) - f(x_{\min})]/D}\,. \tag{5.111}$$

As shown by *Edholm* and *Leimar* [5.25], one can improve (5.111) by calculating the integrals in (5.109) more accurately. By using an expansion in (5.110) up to the fourth term and by evaluating the integrals according to

$$\begin{aligned} \int_{-\infty}^{\infty} \mathrm{e}^{-ax^2+bx^3+cx^4}\mathrm{d}x &\approx \int_{-\infty}^{\infty} \left(1 + bx^3 + cx^4 + \frac{1}{2}b^2x^6\right) \mathrm{e}^{-ax^2}\mathrm{d}x \\ &= \sqrt{\frac{\pi}{a}} \left(1 + \frac{3}{4}\frac{c}{a^2} + \frac{15}{16}\frac{b^2}{a^3}\right), \end{aligned}$$

we get the improved escape rate

$$\begin{aligned} r = r_{\mathrm{K}} \Bigg[1 - D \Bigg(&\frac{1}{8}\frac{f^{(\mathrm{IV})}(x_{\max})}{[f''(x_{\max})]^2} - \frac{1}{8}\frac{f^{(\mathrm{IV})}(x_{\min})}{[f''(x_{\min})]^2} \\ &+ \frac{5}{24}\frac{[f'''(x_{\max})]^2}{|f''(x_{\max})|^3} + \frac{5}{24}\frac{[f'''(x_{\min})]^2}{[f''(x_{\min})]^3} \Bigg) + O(D^2) \Bigg]\,. \end{aligned} \tag{5.112}$$

For the inverted potential $\bar{f}(x) = -f(x)$ we obtain exactly the same escape rates from the well of $\bar{f}$ at $\bar{x}_{\min} = x_{\max}$ over the barrier of $\bar{f}$ at $\bar{x}_{\max} = x_{\min}$.

5.10.2 Bistable and Metastable Potential

Let us now calculate the lowest nonvanishing eigenvalue for the symmetric bistable potential shown in Fig. 5.8a for small diffusion coefficients D. By inverting the potential we get the metastable potential in Fig. 5.8b. The lowest eigenvalue $\bar{\lambda}_0$ of the metastable potential agrees with the lowest nonvanishing eigenvalue $\bar{\lambda}_1$ of the bistable potential, Sect. 5.8. If the Fokker-Planck equation is interpreted as a Smoluchowski equation, the lowest eigenvalue of the metastable potential is the decay rate of particles in the well. In the bistable potential the lowest nonvanishing eigenvalue describes the transition rate between the left and right well.

We first look for the symmetric eigenfunction $\bar{\psi}_0$ and its lowest eigenvalue $\bar{\lambda}_0$ of the metastable potential. For reasons discussed below, we assume that at $x = \pm A$ the potential jumps to a negative infinite value (absorbing wall, Sect. 5.4), so that we have the jump condition (5.84). For further considerations it is useful to transform the eigenvalue equation (5.41) [see (5.35) with $D^{(2)} = D$ and (5.56)]

$$D\frac{\partial}{\partial x}\mathrm{e}^{-\bar{f}(x)/D}\frac{\partial}{\partial x}\mathrm{e}^{\bar{f}(x)/D}\bar{\varphi}_0 = -\bar{\lambda}_0\bar{\varphi}_0 \tag{5.113}$$

into an integral equation. Because of the symmetry of the potential and because the eigenfunction is symmetric $\bar{f}'$ and $\bar{\varphi}_0'$ must be zero at $x = 0$ (i.e., the probability current is zero at $x = 0$), and by integrating (5.113) we obtain

$$D\frac{\partial}{\partial x}\mathrm{e}^{\bar{f}(x)/D}\bar{\varphi}_0 = -\bar{\lambda}_0\mathrm{e}^{\bar{f}(x)/D}\int_0^x \bar{\varphi}_0(z)\,\mathrm{d}z\,.$$

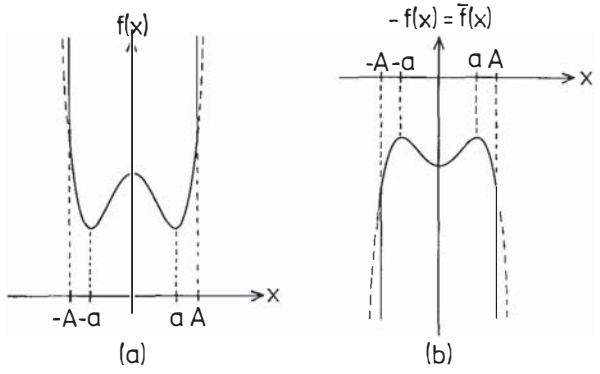

Fig. 5.8. Bistable (**a**) and metastable (**b**) potential

Integrating this equation once more we arrive at the integral equation

$$\bar{\varphi}_0(x) = \mathrm{e}^{-\bar{f}(x)/D}\left[\mathrm{e}^{\bar{f}(0)/D}\bar{\varphi}_0(0) - \frac{\bar{\lambda}_0}{D}\int_0^x \mathrm{d}y\,\mathrm{e}^{\bar{f}(y)/D}\int_0^y \mathrm{d}z\,\bar{\varphi}_0(z)\right]. \tag{5.114}$$

This equation together with the boundary condition

$$\bar{\varphi}_0(A) = 0 \tag{5.115}$$

determines the eigenvalue $\bar{\lambda}_0$ and the eigenfunction $\bar{\varphi}_0$.

For large barrier heights the eigenvalue $\bar{\lambda}_0/D$ will be very small. We may thus apply the following iteration procedure:
As zeroth approximation we use

$$\bar{\varphi}_0^{(0)}(x) = \mathrm{e}^{-\bar{f}(x)/D}\mathrm{e}^{\bar{f}(0)/D}\bar{\varphi}_0(0)\,; \qquad \bar{\lambda}_0^{(0)} = 0\,.$$

If we insert this zeroth approximation into the integral of (5.114) we obtain the first approximation for the eigenfunction

$$\bar{\varphi}_0^{(1)}(x) = \mathrm{e}^{-\bar{f}(x)/D}\mathrm{e}^{\bar{f}(0)/D}\bar{\varphi}_0(0)\left(1 - \frac{\bar{\lambda}_0^{(1)}}{D}\int_0^x \mathrm{d}y\,\mathrm{e}^{\bar{f}(y)/D}\int_0^y \mathrm{d}z\,\mathrm{e}^{-\bar{f}(z)/D}\right). \tag{5.116}$$

Because of (5.115) the eigenvalue $\bar{\lambda}_0$ in first approximation is given by

$$\bar{\lambda}_0^{(1)} = D/\int_0^A \mathrm{d}y\,\mathrm{e}^{\bar{f}(y)/D}\int_0^y \mathrm{d}z\,\mathrm{e}^{-\bar{f}(z)/D}. \tag{5.117}$$

To obtain the eigenfunction and eigenvalue in second order we insert (5.116) in the integral of (5.114) and again use (5.115). Higher approximations are obtained similarly.

For small diffusion coefficients the double integral in (5.117) can be evaluated analytically. For $y = a$ and $z = 0$ there is a very sharp maximum of the integrand $\exp\{[\bar{f}(y) - \bar{f}(z)]/D\}$ for small D. The leading contribution to the double integral stems from the region near this maximum. We therefore expand $\bar{f}(y)$ and $\bar{f}(z)$ around this point ($y = a$, $z = 0$) up to second order, as in (5.110). The integration over y can then be taken from $-\infty$ to $+\infty$ and the integration over z from 0 to $+\infty$. Notice that the double integral factorizes in this approximation, leading to the same integrals as in (5.109) (up to a factor $\frac{1}{2}$ for the first integral). The eigenvalue finally reads

$$\bar{\lambda}_0^{(1)} = \pi^{-1}\sqrt{\bar{f}''(0)\,|\bar{f}''(a)|}\,\mathrm{e}^{-[\bar{f}(a)-\bar{f}(0)]/D} = 2r_{\mathrm{K}}. \tag{5.118}$$

Because we have two barriers in the potential of Fig. 5.8b, it is not surprising that the decay rate $\bar{\lambda}_0$ is twice the Kramers' escape rate over one barrier. We have chosen a finite A in Fig. 5.8b because otherwise the double integral in (5.117)

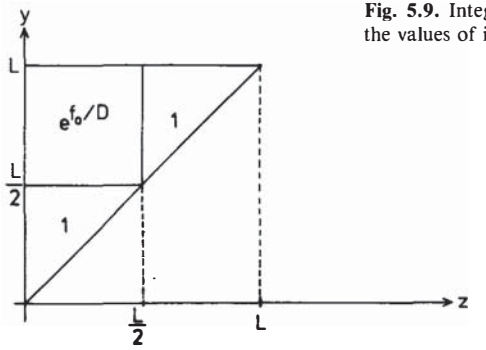

Fig. 5.9. Integration boundary of the double integral and the values of its integrand for the potential in Fig. 5.6

would diverge. As done for the escape rate, (5.118) can be improved by taking into account higher expansion terms of the potential near the maximum and minimum, leading to results in complete agreement with (5.112). (However, $\bar{f}'''(0)$ is now zero because $\bar{f}(x)$ was assumed to be symmetric.)

For the inverted potential of (5.85) (Fig. 5.6) the value of the integrand of the double integral is indicated in Fig. 5.9. The value of the double integral can immediately be read off Fig. 5.9, leading to

$$\bar{\lambda}_0^{(1)} = \frac{4D}{L^2(\mathrm{e}^{f_0/D}+1)} \approx \frac{4D}{L^2}\mathrm{e}^{-f_0/D}, \tag{5.119}$$

which agrees with (5.96) up to the order $\exp(-2f_0/D)$. Neglecting terms of the order $\exp(-3f_0/D)$ we get in second approximation

$$\bar{\lambda}_0^{(2)} = \frac{4D}{L^2}\left(\mathrm{e}^{-f_0/D} - \frac{2}{3}\mathrm{e}^{-2f_0/D}\right), \tag{5.120}$$

which again agrees with (5.96) but now up to the order $\exp(-3f_0/D)$.

Bistable Potential

The same method used for the metastable potential in Fig. 5.8b can be used for the bistable potential in Fig. 5.8a. Because at $x = A$ the probability current must now be zero (reflecting wall, Sect. 5.4), we obtain for the eigenfunction φ_1 the integral equation

$$\varphi_1(x) = \mathrm{e}^{-f(x)/D}\left[\mathrm{e}^{f(A)/D}\varphi_1(A) - \frac{\lambda_1}{D}\int_x^A \mathrm{d}y\,\mathrm{e}^{f(y)/D}\int_y^A \mathrm{d}z\,\varphi_1(z)\right]. \tag{5.121}$$

The eigenfunction φ_1 belonging to the lowest nonvanishing eigenvalue must be an odd function for the bistable potential, i.e.,

$$\varphi_1(0) = 0\,. \tag{5.122}$$

The integral equation (5.121) together with (5.122) determine the eigenfunction φ_1 and the eigenvalue λ_1. We may now apply the same iteration procedure as before. In first order we have

$$\lambda_1^{(1)} = D \Big/ \left(\int_0^A \mathrm{d}y \, \mathrm{e}^{f(y)/D} \int_y^A \mathrm{d}z \, \mathrm{e}^{-f(z)/D} \right). \tag{5.123}$$

It can be shown by partial integration that this expression agrees with (5.117) [notice $f(x) = -\bar{f}(x)$].

Asymmetric Metastable Potential

To treat the asymmetric metastable potential in Fig. 5.10 we need only minor modifications. Because the derivative $\bar{\varphi}_0'(0)$ is no longer zero [$\bar{f}'(0)$ is still zero] instead of the integral equation (5.114) we obtain

$$\bar{\varphi}_0(x) = \mathrm{e}^{-\bar{f}(x)/D} \left[\mathrm{e}^{\bar{f}(0)/D} \bar{\varphi}_0(0) + \int_0^x \mathrm{e}^{\bar{f}(x)/D} \mathrm{d}y \, \bar{\varphi}_0'(0) - \frac{\bar{\lambda}_0}{D} \int_0^x \mathrm{d}y \, \mathrm{e}^{\bar{f}(y)/D} \int_0^y \mathrm{d}z \, \bar{\varphi}_0(z) \right]. \tag{5.124}$$

The eigenfunction $\bar{\varphi}_0$ must vanish at $x = A$ and $x = B$

$$\bar{\varphi}_0(A) = \bar{\varphi}_0(B) = 0 \,. \tag{5.125}$$

To solve (5.124) we may apply the same iteration procedure as before. In zeroth approximation then

$$\bar{\varphi}_0^{(0)}(x) = \mathrm{e}^{-[\bar{f}(x) - \bar{f}(0)]/D} \bar{\varphi}_0(0)$$

$$\bar{\varphi}_0^{(0)\prime}(0) = 0 \,; \qquad \bar{\lambda}_0^{(0)} = 0 \,.$$

Inserting this zeroth solution in the double integral gives

$$\bar{\varphi}_0^{(1)}(x) = \mathrm{e}^{-\bar{f}(x)/D} \mathrm{e}^{\bar{f}(0)/D} \bar{\varphi}_0(0) \left(1 + \int_0^x \mathrm{e}^{\bar{f}(y)/D} \mathrm{d}y \, \alpha - \frac{\bar{\lambda}_0^{(1)}}{D} \int_0^x \mathrm{d}y \, \mathrm{e}^{\bar{f}(y)/D} \int_0^y \mathrm{d}z \, \mathrm{e}^{-\bar{f}(z)/D} \right), \tag{5.126}$$

where α is given by

$$\alpha = \bar{\varphi}_0^{(1)\prime}(0) \, \mathrm{e}^{-\bar{f}(0)/D} / \bar{\varphi}_0(0) \,. \tag{5.127}$$

The two conditions (5.125) then determine α and $\bar{\lambda}_0^{(1)}$. By expanding $f(x)$ near the maxima of the integrands up to second order [as in (5.110)] we obtain

$$\begin{aligned} \bar{\lambda}_0^{(1)} &= (2\pi)^{-1} \left\{ \sqrt{\bar{f}''(0) |\bar{f}''(a)|} \, \mathrm{e}^{-[\bar{f}(a) - \bar{f}(0)]/D} + \sqrt{\bar{f}''(0) |\bar{f}''(b)|} \, \mathrm{e}^{-[\bar{f}(b) - \bar{f}(0)]/D} \right\} \\ &= r_{\mathrm{KR}} + r_{\mathrm{KL}} \,, \end{aligned} \tag{5.128}$$

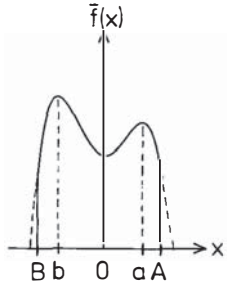

Fig. 5.10. Asymmetric metastable potential

i.e., the sum of the Kramers' escape rates (5.111) over the right and left barriers.

Transformation to a Homogeneous Fredholm Integral Equation

The integral equation (5.114) may be transformed into homogeneous Fredholm integral equation [5.32]. We show this for the metastable potential in Fig. 5.8b. For the bistable potential the expressions are more complicated because the stationary solution must be eliminated first by a projection formalism. Partial integration of (5.114) leads to

$$\bar{\varphi}_0(x) = \mathrm{e}^{-\bar{f}(x)/D} \left\{ \mathrm{e}^{\bar{f}(0)/D} \bar{\varphi}_0(0) + \frac{\bar{\lambda}_0}{D} \left[u(x) \int_0^x \bar{\varphi}_0(y) \, \mathrm{d}y - \int_0^x u(y) \, \bar{\varphi}_0(y) \, \mathrm{d}y \right] \right\}, \tag{5.114a}$$

where we have defined $u(x)$ by

$$u(x) = \int_x^A \exp[\bar{f}(y)/D] \, \mathrm{d}y \,. \tag{5.129}$$

Because of the boundary condition (5.115), i.e.,

$$\bar{\varphi}_0(A) = \mathrm{e}^{-\bar{f}(A)/D} \left[\mathrm{e}^{\bar{f}(0)/D} \bar{\varphi}_0(0) - \frac{\bar{\lambda}_0}{D} \int_0^A u(y) \, \bar{\varphi}_0(y) \, \mathrm{d}y \right] = 0$$

we may write instead of (5.114a)

$$\bar{\varphi}_0(x) = \frac{\bar{\lambda}_0}{D} \mathrm{e}^{-\bar{f}(x)/D} \left[\int_0^x u(x) \, \bar{\varphi}_0(y) \, \mathrm{d}y + \int_x^A u(y) \, \bar{\varphi}_0(y) \, \mathrm{d}y \right].$$

Using instead of the eigenfunction $\bar{\varphi}_0(x)$ the function

$$\bar{\psi}_0(x) = \exp[\bar{f}(x)/(2D)] \, \bar{\varphi}_0(x) \tag{5.130}$$

we obtain the integral equation

$$\bar{\psi}_0(x) = \bar{\lambda}_0 \int_0^A K(x,y)\,\bar{\psi}_0(y)\,\mathrm{d}y \tag{5.131}$$

with the symmetric kernel

$$K(x,y) = K(y,x) = D^{-1}\exp\{-[\bar{f}(x)+\bar{f}(y)]/(2D)\}\cdot\begin{cases} u(x) & \text{for } y<x \\ u(y) & x<y \end{cases}. \tag{5.132}$$

Because we can express the second iterated kernel K_2 in terms of eigenvalues and eigenfunctions of (5.131) [5.2, Chap. III, (58)]

$$K_2(x,z) = \int_0^A K(x,y)K(y,z)\,\mathrm{d}y = \sum_n \bar{\psi}_n(x)\,\bar{\psi}_n(z)/\bar{\lambda}_n^2$$

we obtain

$$\int_0^A K_2(x,x)\,\mathrm{d}x = \int_0^A\int_0^A K(x,y)^2\,\mathrm{d}x\,\mathrm{d}y = \sum_n 1/\bar{\lambda}_n^2. \tag{5.133}$$

If we assume that $\bar{\lambda}_0$ is much smaller than the other eigenvalues

$$0 < \bar{\lambda}_0 \ll \bar{\lambda}_1 < \bar{\lambda}_2 < \ldots \tag{5.134}$$

we get

$$\bar{\lambda}_0 \approx \left[\int_0^A\int_0^A K(x,y)^2\,\mathrm{d}x\,\mathrm{d}y\right]^{-1/2}. \tag{5.135}$$

For small D, $u(x)$ is approximately constant for $x < a$. Then the kernel $K(x,y)$ approximately factorizes and we finally obtain

$$\bar{\lambda}_0 \approx 1/\int_0^A K(x,x)\,\mathrm{d}x = D/\int_0^A \mathrm{e}^{-f(x)/D}\left(\int_x^A \mathrm{e}^{f(y)/D}\mathrm{d}y\right)\mathrm{d}x\,. \tag{5.136}$$

As may be seen by using partial integration this expression agrees with (5.117).

Mean First-Passage Time for the Metastable Potential

The mean first-passage time $T_1(x')$ for a particle starting at $x = x'$ to leave the domain $|x| < A$ can either be obtained by [see (8.5, 9, 10)]

$$T_1(x') = \int_{-A}^A p_1(x,x')\,\mathrm{d}x'\,, \tag{5.137}$$

$$L_{\mathrm{FP}}(x)\,p_1(x,x') = -\delta(x-x')\,, \tag{5.138}$$

$$p_1(\pm A, x') = 0 \tag{5.139}$$

or by, see (8.15a),

$$L_{\mathrm{FP}}^{+}(x')\,T_1(x') = -1\,, \tag{5.140}$$

$$T_1(\pm A) = 0\,. \tag{5.141}$$

For the metastable potential in Fig. 5.8b we now calculate T_1 for $x' = 0$. Because the potential is symmetric and D is independent of x, $p_1(x,0)$ and also $T_1(x')$ must be symmetric in x and x', respectively. Therefore, the first derivative of $p_1(x,0)$ at $x = 0$ and of $T_1(x')$ at $x' = 0$ must vanish. Using

$$\begin{aligned} L_{\mathrm{FP}}(x) &= D\frac{\partial}{\partial x}\mathrm{e}^{-\bar{f}(x)/D}\frac{\partial}{\partial x}\mathrm{e}^{\bar{f}(x)/D} \\ L_{\mathrm{FP}}^{+}(x') &= D\mathrm{e}^{\bar{f}(x')/D}\frac{\partial}{\partial x'}\mathrm{e}^{-\bar{f}(x')/D}\frac{\partial}{\partial x'} \end{aligned} \tag{5.142}$$

it is easy to solve (5.137 – 139):

$$p_1(x,0) = D^{-1}\mathrm{e}^{-\bar{f}(x)/D}\int_x^A \mathrm{e}^{\bar{f}(y)/D}\left[\int_0^y \delta(z)\,\mathrm{d}z\right]\mathrm{d}y\,. \tag{5.143}$$

The δ function in (5.138, 143) may be replaced by a sharp symmetric function of finite width. Then the integral over the δ function for $y > 0$ is 1/2, giving

$$\begin{aligned} T_1(0) &= \int_{-A}^A p_1(x,0)\,\mathrm{d}x = 2\int_0^A p_1(x,0)\,\mathrm{d}x \\ &= D^{-1}\int_0^A \mathrm{e}^{-\bar{f}(x)/D}\left[\int_x^A \mathrm{e}^{\bar{f}(y)/D}\mathrm{d}y\right]\mathrm{d}x\,. \end{aligned} \tag{5.144}$$

The solution of (5.140) with the boundary condition (5.141) and with $\mathrm{d}T_1/\mathrm{d}x'|_{x'=0} = 0$ reads ($|x'| \leqq A$)

$$T_1(x') = D^{-1}\int_{x'}^A \mathrm{e}^{\bar{f}(y)/D}\left(\int_0^y \mathrm{e}^{-\bar{f}(x)/D}\mathrm{d}x\right)\mathrm{d}y\,, \tag{5.145}$$

i.e., for $x' = 0$

$$\begin{aligned} T_1(0) &= D^{-1}\int_0^A \mathrm{e}^{\bar{f}(y)/D}\left(\int_0^y \mathrm{e}^{-\bar{f}(x)/D}\mathrm{d}x\right)\mathrm{d}y \\ &= 1/\bar{\lambda}_0^{(1)}\,. \end{aligned} \tag{5.146}$$

Thus, this expression is equal to the inverse of the first approximation of the eigenvalue, compare (5.117). It is, however, also equal to (5.136, 144) as may be seen by using partial integration.

Thus, for the mean first-passage time an exact expression valid for every potential height and arbitrary diffusion coefficients can be derived. For large potential heights the double integral can be evaluated analytically as done before. The inverse of the mean first-passage time is then given by the sum of the Kramer's escape rates (5.111) over the left and right barriers.