Chapter 7
Exit Problems for Diffusion Processes and Applications

In this chapter, we develop techniques for calculating the statistics of the time that it takes for a diffusion process in a bounded domain to reach the boundary of the domain. We then use this formalism to study the problem of Brownian motion in a bistable potential. Applications such as stochastic resonance and the modeling of Brownian motors are also presented. In Sect. 7.1, we motivate the techniques that we will develop in this chapter by looking at the problem of Brownian motion in bistable potentials. In Sect. 7.2, we obtain a boundary value problem for the mean exit time of a diffusion process from a domain. We then use this formalism in Sect. 7.3 to calculate the escape rate of a Brownian particle from a potential well. The phenomenon of stochastic resonance is investigated in Sect. 7.4. Brownian motors are studied in Sect. 7.5. Bibliographical remarks and exercises can be found in Sects. 7.6 and 7.7, respectively.

7.1 Brownian Motion in a Double-Well Potential

In this section, we study a simple dynamical stochastic system that can exist at two different (meta)stable states. Our goal is to understand how noise enables such a system to jump from one metastable state to another and to calculate how long it will take on average for this transition to occur.

We look at a Brownian particle moving in a double-well potential under the influence of thermal noise in one dimension, the problem that we studied briefly in Sect. 5.2:

$$dX_t = -V'(X_t)\,dt + \sqrt{2\beta^{-1}}\,dW_t, \tag{7.1}$$

with the bistable potential

$$V(x) = \frac{1}{4}x^4 - \frac{1}{2}x^2 + \frac{1}{4}. \tag{7.2}$$

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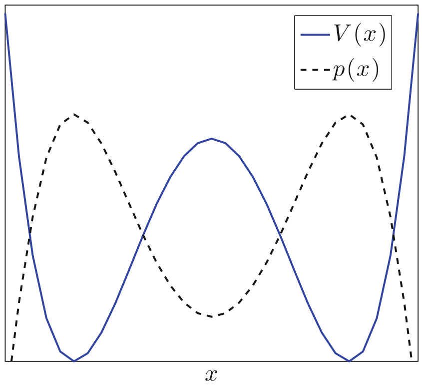

Fig. 7.1 Bistable potential (7.2) and invariant distribution (7.4)

This potential has three extrema: a local maximum at $x = 0$ and two local minima at $x = \pm 1$. The values of the potential at these three points are $V(\pm 1) = 0$, $V(0) = \frac{1}{4}$. We will say that the height of the potential barrier is $\Delta V = \frac{1}{4}$. We are interested in understanding the dynamics (7.1) in the asymptotic regime where the thermal fluctuations, whose strength is measured by the temperature β^{-1}, are weak compared to the potential barrier ΔV:

$$\frac{1}{\beta \Delta V} \ll 1. \tag{7.3}$$

As we have already seen, the dynamics (7.1) is ergodic with respect to the distribution

$$\rho_s(x) = \frac{1}{Z} e^{-\beta V(x)}. \tag{7.4}$$

At low temperatures, $\beta \gg 1$, most of mass of the invariant distribution is concentrated around the minima of the potential; see Fig. 7.1. It is expected that stationery trajectories of X_t will spend most time oscillating around the two local minima of the potential, while occasionally hopping between the two local minima of the potential. This intuition is confirmed by performing numerical simulations; see Fig. 7.2. This is a noise-assisted event: in the absence of noise, the process X_t ends up at one of the two minima of the potential, depending on its initial condition. Indeed, it is easy to check that the potential itself is a Lyapunov function for the deterministic dynamics. For the noise dynamics, we will refer to the two local minima of the potential as *metastable states*.

The time that it takes for the "particle" X_t to acquire a sufficient amount of energy from the noise so that it can surmount the potential barrier ΔV and escape from one of the metastable states depends on the strength of the noise, i.e., the temperature. When the noise is weak, the particle spends a long time at the metastable state (relative to the time scale introduced by Assumption 7.3), before being able to escape from it. This is an example of a *rare event*. The relevant time scale, the *mean exit time* or the *mean first passage time*, scales exponentially in β:

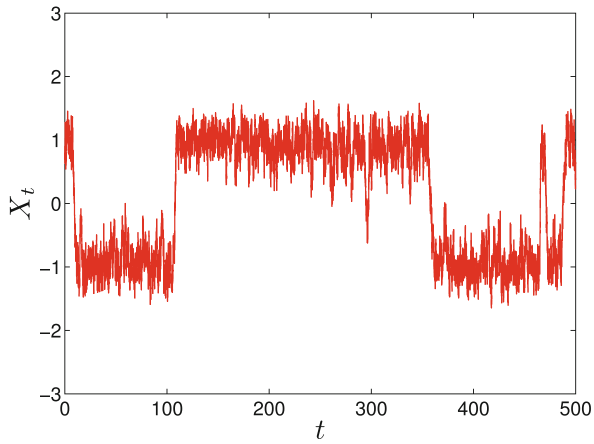

Fig. 7.2 Sample path of X_t, the solution of (7.1) with the bistable potential (7.2)

$$\tau = \nu^{-1} \exp(\beta \Delta V). \tag{7.5}$$

We will refer to this as the *Kramers time*. The inverse of the Kramers time is proportional to the *reaction rate* (hopping rate) $\kappa \sim \tau^{-1}$, which gives the rate at which particles escape from a local minimum of the potential:

$$\kappa \sim \nu \exp(-\beta \Delta V). \tag{7.6}$$

The prefactor ν is called the *rate coefficient*. This hopping mechanism between metastable states becomes less pronounced at higher temperatures. For β sufficiently low, the dynamics (7.1) is dominated by noise, and transitions between the two metastable states cease to be rare events.

One of our goals in this chapter will be to obtain (7.5) in a systematic way and furthermore, to obtain a formula for the prefactor ν. More generally, we want to consider stochastic dynamical systems of the form (7.1) that possess several metastable states. We want to characterize transitions between these states and to calculate transition rates. This will be done in Sects. 7.2 and 7.3. Later in this chapter, we will also consider the effect of adding a time-periodic external forcing to stochastic systems with metastable states. This will be done in Sects. 7.4 and 7.5.

7.2 The Mean Exit Time

In order to calculate the hopping rate κ for the dynamics (7.1) in a metastable potential (7.2), we need to calculate the time it takes on average for the diffusion process X_t to escape from one of the local minima of the potential, or more generally, the time it takes on average for a diffusion process to escape from a metastable state. This *mean exit time* from a metastable state is an example of a *mean first passage* *time* (MFPT): we want to calculate how long it takes on average for a diffusion process to reach the boundary of a domain. When the domain is the basin of attraction of one of the local minima of the potential, the mean first passage time gives us the average time it takes for the diffusing particle to reach the local maximum of the potential.

We can calculate the mean exit time τ for a diffusion process X_t in a systematic way by showing that it is the solution of a boundary value problem that involves the generator of the process X_t. This boundary value problem, see equation (7.9), can be justified rigorously using Dynkin's formula (3.110). In this section, we present a formal derivation of this equation that will be sufficient for our purposes.

The Boundary Value Problem for the Mean Exit Time

Let X_t^x denote the solution of the stochastic differential equation

$$dX_t^x = b(X_t^x)\,dt + \sigma(X_t^x)\,dW_t, \quad X_0^x = x, \tag{7.7}$$

in $\mathbb{R}^d$, and let D be a bounded subset of $\mathbb{R}^d$ with smooth boundary. We have introduced the superscript x to emphasize the dependence of the solution to the SDE on the initial point x. Given $x \in D$, we define the *first passage time* or *first exit time* to be the first time that X_t^x exits the domain D:

$$\tau_D^x = \inf\{t \geqslant 0 : X_t^x \notin D\}.$$

This is an example of a *stopping time* (see Sect. 3.8): the information that we have about our stochastic process up to time t is sufficient to determine whether the event $\tau \leqslant t$ has occurred. The average of this random variable is called the mean first passage time or the mean exit time:

$$\tau(x) := \mathbb{E}\tau_D^x = \mathbb{E}\left(\inf\{t \geqslant 0 : X_t^x \notin D\} \middle| X_0^x = x\right).$$

We have written the second equality in the above in order to emphasize the fact that the mean first passage time is defined in terms of a conditional expectation, i.e., the mean exit time is defined as the expectation of the first time the diffusion processes X_t leaves the domain, conditioned on X_t starting at $x \in \Omega$. Consequently, the mean exit time is a function of the starting point x. Consider now an ensemble of initial conditions distributed according to a distribution $p_0(x)$. The *confinement time* is defined as

$$\bar{\tau} = \int_\Omega \tau(x) p_0(x)\,dx = \int_\Omega \mathbb{E}\left(\inf\{t \geqslant 0 : X_t^x \notin D\} \middle| X_0^x = x\right) p_0(x)\,dx. \tag{7.8}$$

We can calculate the mean exit time by solving an appropriate boundary value problem. The calculation of the confinement time follows, then, by calculating the integral in (7.8).

Result 7.1 *The mean exit time is given by the solution of the boundary value problem*

$$-\mathscr{L}\tau = 1, \quad x \in D, \tag{7.9a}$$

$$\tau = 0, \quad x \in \partial D, \tag{7.9b}$$

where $\mathscr{L}$ is the generator of the diffusion process 7.7.

The homogeneous Dirichlet boundary conditions correspond to an absorbing boundary: the particles are removed when they reach the boundary. Other choices of boundary conditions are also possible; see Eq. (7.11).

Derivation of Result 7.1. Let $\rho(y,t|x)$ be the probability distribution of the particles that *have not left* the domain D at time t. It satisfies the Fokker–Planck equation with absorbing boundary conditions:

$$\frac{\partial \rho}{\partial t} = \mathscr{L}^* \rho, \quad \rho(y,0|x) = \delta(y-x), \quad \rho|_{\partial D} = 0, \tag{7.10}$$

where $\mathscr{L}^*$ is a differential operator in y. We can write the solution to this equation in the form

$$\rho(y,t|x) = e^{\mathscr{L}^* t}\delta(y-x),$$

where the absorbing boundary conditions are included in the definition of the semigroup $e^{\mathscr{L}^* t}$. The homogeneous Dirichlet (absorbing) boundary conditions imply that

$$\lim_{t \to +\infty} \rho(y,t|x) = 0.$$

That is, all particles will eventually leave the domain. The (normalized) number of particles that are still inside D at time t is

$$S(x,t) = \int_D \rho(y,t|x)\,dy.$$

Note that this is a decreasing function of time. We can write

$$\frac{\partial S}{\partial t} = -f(x,t),$$

where $f(x,t)$ is the *first passage time distribution*. The mean exit time is the first moment of the distribution $f(x,t)$:

$$\begin{aligned}
\tau(x) &= \int_0^{+\infty} f(x,s) s\,ds = \int_0^{+\infty} -\frac{dS}{ds} s\,ds \\
&= \int_0^{+\infty} S(s,x)\,ds = \int_0^{+\infty} \int_D \rho(y,s|x)\,dyds \\
&= \int_0^{+\infty} \int_D e^{\mathscr{L}^* s}\delta(y-x)\,dyds \\
&= \int_0^{+\infty} \int_D \delta(y-x)\left(e^{\mathscr{L} s}1\right) dyds = \int_0^{+\infty} \left(e^{\mathscr{L} s}1\right)(x)\,ds.
\end{aligned}$$

We apply $\mathscr{L}$ to the above equation to deduce

$$\mathscr{L}\tau = \int_0^{+\infty} \left(\mathscr{L}e^{\mathscr{L}t}1\right) dt = \int_0^{+\infty} \frac{d}{dt}\left(e^{\mathscr{L}t}1\right) dt$$
$$= -1.$$

□

When a part of the boundary is absorbing and a part is reflecting, then we end up with a mixed boundary value problem for the mean exit time:

$$-\mathscr{L}\tau = 1, \quad x \in D, \tag{7.11a}$$
$$\tau = 0, \quad x \in \partial D_A, \tag{7.11b}$$
$$\eta \cdot \mathbf{J} = 0, \quad x \in \partial D_R. \tag{7.11c}$$

Here $\partial D_A \cup \partial D_R = \partial D$, where $\partial D_A \neq \emptyset$ denotes the absorbing part of the boundary, ∂D_R denotes the reflecting part, and $\mathbf{J}$ denotes the probability flux.

7.2.1 *Examples*

We can study now a few simple examples for which we can calculate the mean first passage time in closed form.

Brownian Motion with One Absorbing and One Reflecting Boundary

We consider the problem of Brownian motion (with diffusion coefficient 2) moving in the interval $[a,b]$. We assume that the left boundary is absorbing and the right boundary is reflecting. The boundary value problem for the mean exit time becomes

$$-\frac{d^2\tau}{dx^2} = 1, \quad \tau(a) = 0, \ \frac{d\tau}{dx}(b) = 0. \tag{7.12}$$

The solution of this equation is

$$\tau(x) = -\frac{x^2 - a^2}{2} + b(x - a).$$

The mean exit time for Brownian motion with one absorbing and one reflecting boundary in the interval $[-1,1]$ is plotted in Fig. 7.3a.

Brownian Motion with Two Absorbing Boundaries

Consider again the problem of Brownian motion with diffusion coefficient 2 moving in the interval $[a,b]$, but now with both boundaries absorbing. The boundary value problem for the MFPT time becomes

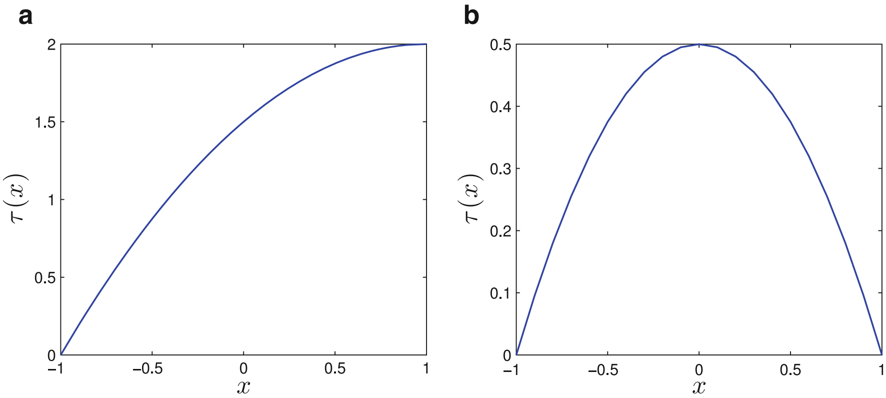

Fig. 7.3 The mean exit time for Brownian motion with one absorbing and one reflecting boundary (**a**) and two absorbing boundaries (**b**)

$$-\frac{d^2\tau}{dx^2} = 1, \quad \tau(a) = 0, \ \tau(b) = 0. \tag{7.13}$$

The solution of this equation is

$$\tau(x) = -\frac{x^2}{2} + \frac{a+b}{2}x - \frac{ab}{2}.$$

The MFPT time for Brownian motion with two absorbing boundaries in the interval $[-1,1]$ is plotted in Fig. 7.3b.

The Mean First Passage Time for a One-Dimensional Diffusion Process

Consider now the mean exit time problem from an interval $[a,b]$ for a general one-dimensional diffusion process with generator

$$\mathscr{L} = b(x)\frac{d}{dx} + \frac{1}{2}\Sigma(x)\frac{d^2}{dx^2},$$

where the drift and diffusion coefficients are smooth functions and where the diffusion coefficient $\Sigma(x)$ is a strictly positive function (uniform ellipticity condition). In order to calculate the mean first passage time, we need to solve the differential equation

$$-\left(b(x)\frac{d}{dx} + \frac{1}{2}\Sigma(x)\frac{d^2}{dx^2}\right)\tau = 1, \tag{7.14}$$

together with appropriate boundary conditions, depending on whether we have one absorbing and one reflecting boundary or two absorbing boundaries. To solve this equation, we first define the function $\psi(x)$ through $\psi'(x) = 2b(x)/\Sigma(x)$ to write (7.14) in the form

$$\left(e^{\psi(x)}\tau'(x)\right)' = -\frac{2}{\Sigma(x)}e^{\psi(x)}.$$

The general solution of (7.14) is obtained after two integrations:

$$\tau(x) = -2\int_a^x e^{-\psi(z)}\,dz \int_a^z \frac{e^{\psi(y)}}{\Sigma(y)}\,dy + c_1 \int_a^x e^{-\psi(y)}\,dy + c_2,$$

where the constants c_1 and c_2 are to be determined from the boundary conditions. When both boundaries are absorbing, we get

$$c_1 = \frac{2\int_a^b e^{-\psi(z)}\,dz \int_a^z \frac{e^{\psi(y)}}{\Sigma(y)}\,dy}{\int_a^b e^{-\psi(y)}\,dy}, \quad c_2 = 0,$$

whereas when the left boundary is absorbing and the right is reflecting, we have

$$c_1 = 2\int_a^b \frac{e^{\psi(y)}}{\Sigma(y)}\,dy, \quad c_2 = 0.$$

7.3 Escape from a Potential Well

Now we can use the theory developed in the previous section to calculate the escape rate and the mean exit time from a metastable state for a particle moving in a double-well potential of the form (7.2) for the overdamped Langevin dynamics (7.1).

We assume that the left and right minima of the potential are located at $x = a$ and $x = c$, respectively; the local maximum is at $x = b$, $a < b < c$. We will calculate the rate of escape from the left minimum. For this, we need to know how long it will take, on average, for a particle starting close to the minimum a to reach the local maximum.

We assume that the particle is initially at x_0, which is near a. The boundary value problem for the mean exit time from the interval (a,b) for the one-dimensional diffusion process (7.1) reads

$$-\beta^{-1} e^{\beta V} \frac{d}{dx}\left(e^{-\beta V} \frac{d}{dx}\tau\right) = 1. \tag{7.15}$$

In view of the fact that the particle cannot move too much to the left, since the potential is confining, we choose reflecting boundary conditions at $x = a$. We also choose absorbing boundary conditions at $x = b$, since we are assuming that the particle escapes the left minimum when it reaches the point b. We can solve (7.15) with these boundary conditions by quadratures:

$$\tau(x) = \beta \int_x^b dy e^{\beta V(y)} \int_a^y dz e^{-\beta V(z)}. \tag{7.16}$$

The potential grows sufficiently fast at infinity to allow us to replace the boundary conditions at $x = a$ by a repelling/reflecting boundary condition at $x = -\infty$:[1]

[1] In other words, the integral $\int_{-\infty}^a e^{-\beta V(y)}\,dy$ can be neglected.

$$\tau(x) \approx \beta \int_x^b dy e^{\beta V(y)} \int_{-\infty}^y dz e^{-\beta V(z)}.$$

When $\Delta V \beta \gg 1$, the integral with respect to z is dominated by the value of the potential near a. We can use the Taylor series expansion around the minimum:

$$V(z) = V(a) + \frac{1}{2}\omega_a^2 (z-a)^2 + \cdots$$

Furthermore, we can replace the upper limit of integration by $+\infty$:

$$\int_{-\infty}^{y} e^{-\beta V(z)} \, dz \approx \int_{-\infty}^{+\infty} e^{-\beta V(a)} e^{-\frac{\beta\omega_a^2}{2}(z-a)^2} \, dz$$
$$= e^{-\beta V(a)} \sqrt{\frac{2\pi}{\beta\omega_a^2}}.$$

Similarly, the integral with respect to y is dominated by the value of the potential around the local maximum b. We use the Taylor series expansion

$$V(y) = V(b) - \frac{1}{2}\omega_b^2 (y-b)^2 + \cdots .$$

Assuming that x is close to the left local minimum a, we can replace the lower limit of integration by $-\infty$. We have

$$\int_x^b e^{\beta V(y)} \, dy \approx \int_{-\infty}^{b} e^{\beta V(b)} e^{-\frac{\beta\omega_b^2}{2}(y-b)^2} \, dy$$
$$= \frac{1}{2} e^{\beta V(b)} \sqrt{\frac{2\pi}{\beta\omega_b^2}}.$$

Putting everything together, we obtain the following formula for the mean exit time:

$$\tau = \frac{\pi}{\omega_a \omega_b} e^{\beta \Delta V}. \tag{7.17}$$

This is independent of the point x, provided that it is close to the local minimum a.

The rate of arrival at the local maximum b is $1/\tau$. Once a particle has reached b, it has a 50% chance of moving to the left and a 50% of moving to the right. In other words, only half of the particles that reach b manage to escape. Consequently, the escape rate (or reaction rate) for x in the vicinity of a is given by $\frac{1}{2\tau}$:

$$\kappa = \frac{\omega_a \omega_b}{2\pi} e^{-\beta \Delta V}. \tag{7.18}$$

We will refer to (7.17) as the *Kramers time* and to (7.18) as the *Kramers rate*.

Example 7.1. We can approximate a double-well potential of the form (7.2) by either a piecewise linear or a piecewise constant potential. Consider a symmetric bistable potential with minima at $x = \pm L$ and maximum at $x = 0$. We consider the piecewise linear potential

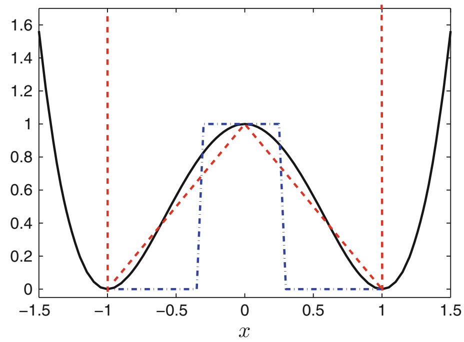

Fig. 7.4 Piecewise linear and piecewise constant approximations of a symmetric double-well potential

$$V_L(x) = \begin{cases} \frac{\delta}{L}(L-x) & x \in [0,L], \\ \frac{\delta}{L}(L+x) & x \in [-L,0], \\ +\infty & x \notin [-L,L], \end{cases} \tag{7.19}$$

The constant $\delta > 0$ is chosen so that we get the best fit of the double-well potential. Similarly, we can also consider the piecewise constant approximation

$$V_C(x) = \begin{cases} 0 & x \in [\alpha,L], \\ \zeta & x \in [-\alpha,\alpha], \\ 0 & x \in [-L,-\alpha], \\ +\infty & x \notin [-L,L]. \end{cases} \tag{7.20}$$

Again, the constants $\zeta, \alpha > 0$ are chosen to obtain the best fit. These approximations are compared to a symmetric double-well potential in Fig. 7.4.

Using formula (7.16), we can obtain an analytical expression for the mean exit time from the left well for the piecewise linear potential (7.19). We have the following:[2]

$$\begin{aligned} \tau(x) &= \beta \int_x^0 dy e^{\beta \frac{\delta}{L}(L+y)} \int_{-L}^{y} dz e^{-\beta \frac{\delta}{L}(L+z)} \\ &= \frac{Lx}{\delta} + \frac{L^2}{\beta \delta^2}\left(e^{\beta\delta} - e^{\frac{\beta\delta}{L}(x+L)}\right), \end{aligned} \tag{7.21}$$

for $x \in [-L,0]$.

In Fig. 7.5a, we use (7.21) (for $\delta = L = 1$) to plot the mean exit time from the left well for a particle starting at the bottom of the well as a function of the temperature. In Fig. 7.5b, we plot the mean exit time from the left well as a function of the starting point for different values of the temperature. As expected, the mean exit time decreases exponentially fast as the temperature increases. Furthermore, the mean exit time decreases rapidly in a layer close the the local maximum $x = 0$.

[2] The boundary conditions are reflecting at $x = -L$ and absorbing at $x = 0$, whence (7.16) is the correct formula to use.

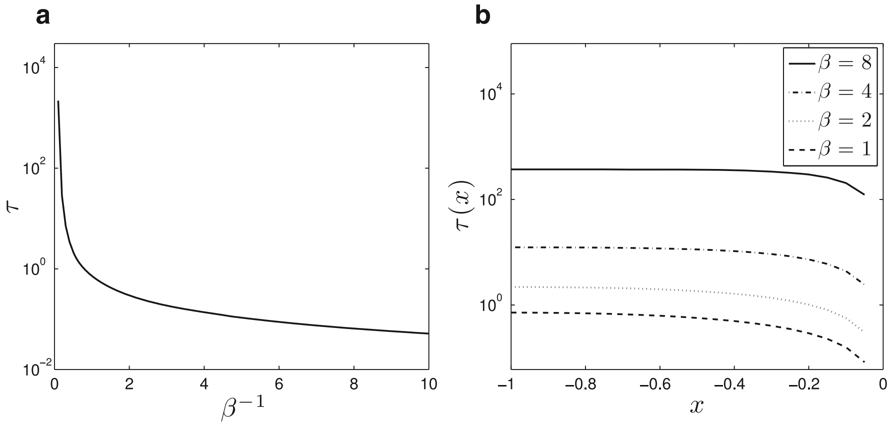

Fig. 7.5 Mean exit time for a particle starting at $x \in [-L, 0]$ for the piecewise linear potential. (**a**): τ as a function of temperature; (**b**): τ as a function of x for different values of the temperature β^{-1}

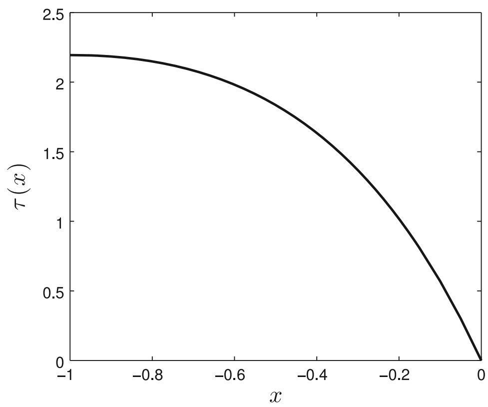

Fig. 7.6 Mean exit time for a particle starting at $x \in [-L, 0]$ for the piecewise linear potential at inverse temperature $\beta = 2$

This phenomenon becomes more pronounced for lower values of the temperature. Similar results can be obtained for the piecewise constant potential; see Exercise 1.

7.4 Stochastic Resonance

In this section, we study the effect of adding a time-periodic forcing to the dynamics (7.1). In particular, we are interested in understanding the effect that the time-dependent forcing has on the hopping rate between the two wells of the potential and on whether it can induce a coherent response of the system in the presence of noise.