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On the length of one-dimensional reactive paths

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Abstract. Motivated by some numerical observations on molecular dynamics simulations, we analyze metastable trajectories in a very simple setting, namely paths generated by a one-dimensional overdamped Langevin equation for a double well potential. Specifically, we are interested in so-called reactive paths, namely trajectories which leave definitely one well and reach the other one. The aim of this paper is to precisely analyze the distribution of the lengths of reactive paths in the limit of small temperature, and to compare the theoretical results to numerical results obtained by a Monte Carlo method, namely the multi-level splitting approach (see Cérou et al. (2011)).

1. Introduction and main results

1.1. *Motivation and presentation of reactive paths.* A prototypical example of a dynamics which is used to describe the evolution of a molecular system is the so-called overdamped Langevin dynamics:

$$dX_t^{(\varepsilon)} = -\nabla V\left(X_t^{(\varepsilon)}\right) dt + \sqrt{2\varepsilon}dB_t, \tag{1.1}$$

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where $X_t^{(\varepsilon)} \in \mathbb{R}^d$ denotes the position of the particles (think of the nuclei of a molecule), $V : \mathbb{R}^d \to \mathbb{R}$ is the given potential function modeling the interaction between the particles, $(B_t)_{t\geq 0}$ is a standard Brownian motion on $\mathbb{R}^d$ and ε is a (small) positive parameter proportional to temperature. The potential V is assumed to be smooth and to grow sufficiently fast to infinity at infinity so that the stochastic differential equation (1.1) admits a unique strong solution. One common feature of many molecular dynamics simulations is that the dynamics (1.1) is metastable: the stochastic process $\left(X_t^{(\varepsilon)}\right)_{t\geq 0}$ spends a lot of time in some region before hopping to another region. These hopping events are exactly those of interest, since they are associated to large changes of conformations of the molecular system, which can be seen at the macroscopic level.

In the following, we focus on the limit of small temperature (namely ε goes to zero). In this case, the Freidlin-Wentzell theory (see Freidlin and Wentzell (1998)) is very useful to understand these hopping events. Specifically, it turns out that the metastable states are neighborhoods of the local minima of the potential V, and that the time it takes to leave a metastable state to reach another one is of the order of

$$C \exp(\delta V/\varepsilon). \tag{1.2}$$

Here, δV is the height of the barrier to be overcome (namely the difference in energy between the saddle point and the initial local minimum), and C is a constant depending on the eigenvalues of the Hessian of the potential at the minimum and at the saddle point (see Equation (1.3) below for a precise formula in the one-dimensional case). This is the so-called Eyring-Kramers (or Arrhenius) law, and we refer for example to Bovier et al. (2004); Berglund (2011); Menz and Schlichting (2012) for more precise results.

Actually, the most interesting part of a transition path between two metastable states is the final part, namely the piece of the trajectory which definitely leaves the initial metastable state and then goes to the next metastable region: this is the so-called *reactive trajectory* (or *reactive path*), see Hummer (2004); E and Vanden-Eijnden (2004) and Lu and Nolen (2013) for a recent mathematical analysis of such paths. In particular, reactive paths provide relevant information on the transition states between the two metastable states. One numerical challenge in molecular dynamics is thus to be able to efficiently sample these reactive paths. Notice that from the Eyring-Kramers law (1.2), a naive Monte Carlo method (which means, generating trajectories according to (1.1) and waiting for a transition event) cannot provide efficiently a large sample of reactive paths, hence the need for dedicated algorithms.

In Cérou et al. (2011), we proposed a numerical method based on an adaptive multilevel splitting algorithm to sample reactive trajectories. One interesting observation we made is that the lengths of these reactive paths seem to behave very differently from (1.2), see Figure 1.2 below. It seems that, in the limit of small ε, the distribution of these lengths is a fixed distribution shifted by an additive factor $-\log \varepsilon$. The aim of this work is to use analytical tools to precisely analyze this distribution in the asymptotic regime ε goes to zero, and to give a proof of this numerical observation.

1.2. *The one-dimensional setting and our main results.* In the following, we consider a one-dimensional case ($d = 1$), and we assume (for simplicity) that the potential V admits exactly two local minima (V is a double-well potential). Specifically, let us denote $x^* < y^*$ the two local minima of V and $z^* \in (x^*, y^*)$ the point where V reaches its local maximum in between. As explained above, we are interested in trajectories solution to (1.1) from x^* to y^*, and more precisely in the end of the path from x^* to y^* (the reactive paths). In order to precisely define these reactive paths, let us introduce the first hitting time of a ball centered at y^* with (small) radius $\delta_y > 0$, starting from x^*:

$$T_{y^*}^{x^*} = \inf\Big\{t > 0 \,:\, |X_t^{(\varepsilon)} - y^*| < \delta_y\Big\} \quad \text{with } X_0^{(\varepsilon)} = x^*.$$

In this setting, formula (1.2) writes (notice that $V''(x^*) > 0$ and $V''(z^*) < 0$):

$$\mathbb{E}\Big(T_{y^*}^{x^*}\Big) \underset{\varepsilon\to 0}{\sim} \frac{2\pi}{\sqrt{V''(x^*)|V''(z^*)|}} \exp\left((V(z^*) - V(x^*))/\varepsilon\right). \tag{1.3}$$

The d-dimensional version of this result is established in Bovier et al. (2004). Let us also introduce the last exit time from the ball centered at x^* with (small) radius $\delta_x > 0$ before the time $T_{y^*}^{x^*}$ (again starting from $X_0^{(\varepsilon)} = x^*$):

$$S_{y^*}^{x^*} = \sup\Big\{t < T_{y^*}^{x^*} \,:\, |X_t^{(\varepsilon)} - x^*| < \delta_x\Big\}.$$

The question we would like to address is: how long is a reactive path, that is the time $T_{y^*}^{x^*} - S_{y^*}^{x^*}$ as ε goes to 0?

This question was partially addressed in Freidlin and Wentzell (1998) where the ball centered around y^* is replaced by the complementary of the domain of attraction of x^* for the deterministic dynamical system corresponding to (1.1) with $\varepsilon = 0$. Several papers are dedicated to the more subtle situation where points on the boundary of this domain are not attracted to x^*. In our simple framework, such a domain is given by $(-\infty, z^*)$ (see Maier and Stein (1997) for such a study). In Day (1990, 1992, 1995), the author is interested in the law of the exit time from a domain containing an unstable equilibrium when the diffusion starts on the stable manifold (see also Berglund and Gentz (2004); Bakhtin (2008)). Up to a translation term, these exit times converge to a random variable of law $-\log|N|$ where N is a standard Gaussian variable. The probability density function of such a random variable is given by

$$x \mapsto \sqrt{\frac{2}{\pi}} \exp\left(-x - \frac{1}{2}e^{-2x}\right).$$

This is not the one of a Gumbel variable (see (1.7)). Nevertheless this Gumbel distribution also appears for example in Proposition 3.3 in Day (1992). Note also that similar questions can be formulated in a discrete context (see for example Schonmann (1992)).

In order to specify our purpose, let us now make our assumptions on the potential V more precise.

Assumption 1.1. The potential V is smooth, has exactly two local minima $x^* < 0$ and $y^* > 0$ and a local maximum $z^* = 0$. Moreover, V' is positive on $(x^*, 0)$ and negative on $(0, y^*)$ and the local maximum at 0 is assumed to be non-degenerate:

$$V(0) = 0, \quad V'(0) = 0, \quad \text{and} \quad V''(0) = -\alpha < 0. \tag{1.4}$$

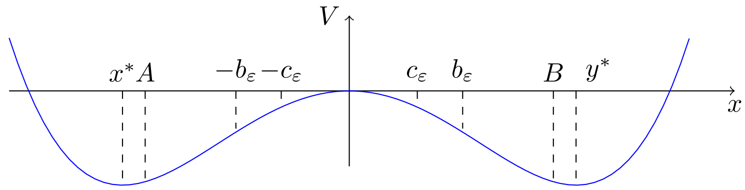

FIGURE 1.1. Shape of the potential V defined in (1.6). The points $\pm b_\varepsilon$ and $\pm c_\varepsilon$ go to 0 as $\varepsilon \to 0$.

Notice that the potential V is close to $x \mapsto -\alpha x^2/2$ for values of x around 0. More precisely, it is easy to show that there exist $K > 0$ and $\delta > 0$ such that, for all $|x| < \delta$,

$$-Kx^2 \leq V'(x) + \alpha x \leq Kx^2 \quad \text{and} \quad -\frac{K|x|^3}{3} \leq V(x) + \frac{\alpha x^2}{2} \leq \frac{K|x|^3}{3}. \tag{1.5}$$

Example 1.2. An example of a potential which satisfies Assumption 1.1 is (see also Figure 1.1)

$$V:\ x \mapsto \frac{x^4}{4} - \frac{x^2}{2}. \tag{1.6}$$

In this case, -1 and $+1$ are the two (global) minima. This is a double well potential with a local maximum at $x = 0$ which is non degenerate, with $\alpha = 1$.

Let us denote $A = x^* + \delta_x \in (x^*, 0)$, $B = y^* - \delta_y \in (0, y^*)$ and $x \in (A, 0)$. We are interested in the behavior of

$$T_{x\to B} = \inf\left\{t > 0\ :\ X_t^{(\varepsilon)} = B\right\} \quad \text{cond. to the event } \left\{X_0^{(\varepsilon)} = x,\ T_B < T_A\right\},$$

when ε goes to zero. At the end of the day, the aim is to let x go to A. As mentioned above, simulations in Cérou et al. (2011) suggest that, if the local maximum is non degenerated, then the law of this length looks like a fixed law shifted as ε goes to 0. Figure 1.2 presents the density of the reactive path $T_{x\to B}$ for several values of ε, when $V(x) = x^4/4 - x^2/2$, $A = -0.9$, $B = 0.9$, and $x = -0.89$. In Cérou et al. (2011); Luccioli et al. (2010), it is suggested that the asymptotic shape of these laws is an Inverse Gaussian distribution. In fact, it is not the case: it turns out to be a Gumbel distribution.

Definition 1.3 (Standard Gumbel distribution)**.** The standard Gumbel distribution is defined by its density function

$$f(x) = \exp\left(-x - e^{-x}\right). \tag{1.7}$$

Its Laplace transform is given by

$$\mathbb{E}\left(e^{-sG}\right) = \begin{cases} \Gamma(1+s) & \text{if } s > -1, \\ +\infty & \text{otherwise,} \end{cases}$$

where $\Gamma(z) = \int_0^\infty t^{z-1} e^{-t}\, dt$ is the Euler's Gamma function.

The main result of the paper is the following convergence in distribution.

Theorem 1.4. *Under Assumption 1.1, for any $A \in (x^*, 0)$, $B \in (0, y^*)$, and $x \in (A, 0)$ we have, conditionally to the event $\left\{X_0^{(\varepsilon)} = x,\ T_B < T_A\right\}$,*

$$T_{x\to B} + \frac{1}{\alpha}\log\varepsilon \xrightarrow[\varepsilon\to 0]{\mathcal{L}} \frac{1}{\alpha}(\log(|x|B) + F(x) + F(B) - \log\alpha + G)$$

where G is a standard Gumbel random variable and

$$F(s) = \int_s^0 \left(\frac{\alpha}{V'(t)} + \frac{1}{t}\right) dt$$

for any $s \in (x^*, y^*)$.

Notice that by (1.4), the integral defining the function F is well defined. We slightly abuse notation and denote $T_{A\to B}$ the limit of $T_{x\to B}$ when x goes to A. We then have

$$T_{A\to B} + \frac{1}{\alpha}\log\varepsilon \xrightarrow[\varepsilon\to 0]{\mathcal{L}} \frac{1}{\alpha}(\log(|A|B) + F(A) + F(B) - \log\alpha + G).$$

Example 1.5. Let us come back to our previous example where the potential V is defined as

$$V:\ x \mapsto \frac{x^4}{4} - \frac{x^2}{2}.$$

In this case, $\alpha = 1$ and if we choose $A = -0.9$, $B = 0.9$, and $x = -0.89$, we get

$$T_{-0.89\to 0.9} + \log\varepsilon \xrightarrow[\varepsilon\to 0]{\mathcal{L}} \log(0.89\times 0.9) - \frac{1}{2}\log(1-0.89^2) - \frac{1}{2}\log(1-0.9^2) + G.$$

This is illustrated on the left hand side of Figure 1.2 and on Figure 4.4 below.

The paper is organized as follows. Section 2 recalls classical tools that are used in the proofs. Section 3 provides a key estimate for the (repulsive) Ornstein-Uhlenbeck process. The proof of Theorem 1.4 is given in Section 4. Finally, Section 5 is devoted to particular potentials that are degenerated at the origin (*i.e.*, $V''(0) = 0$) or singular (*e.g.*, $V(x) = -|x|$).

2. Classical tools

2.1. *Laplace transform of the exit time.* Let us first recall how one can link the Laplace transform of the exit time of an interval to the infinitesimal generator A_ε of the diffusion process (1.1) where

$$A_\varepsilon f(x) = \varepsilon f''(x) - V'(x)f'(x).$$

Fix $a < x < b$ and denote by $H_{a,b}^{(\varepsilon)}$ the first exit time from (a,b), starting from x:

$$H_{a,b}^{(\varepsilon)} = \inf\left\{t > 0\ :\ X_t^{(\varepsilon)} \notin (a,b)\right\} = T_a^{(\varepsilon)} \wedge T_b^{(\varepsilon)},$$

where

$$T_c^{(\varepsilon)} = \inf\left\{t > 0\ :\ X_t^{(\varepsilon)} = c\right\}.$$

In the sequel, for the ease of notation, we may sometimes drop the superscript ε and the indices a and b. For example, we will denote H for $H_{a,b}^{(\varepsilon)}$.

Notice that $\left\{X_H^{(\varepsilon)} = b\right\} = \{T_b < T_a\}$. For any $s \in [0, +\infty)$ and $x \in (a,b)$, let us define

$$F_\varepsilon(s,x) := \mathbb{E}_x\left(e^{-sH}|X_H^{(\varepsilon)} = b\right) \quad \text{and} \quad F_\varepsilon(s) = \lim_{x\to a} F_\varepsilon(s,x), \tag{2.1}$$

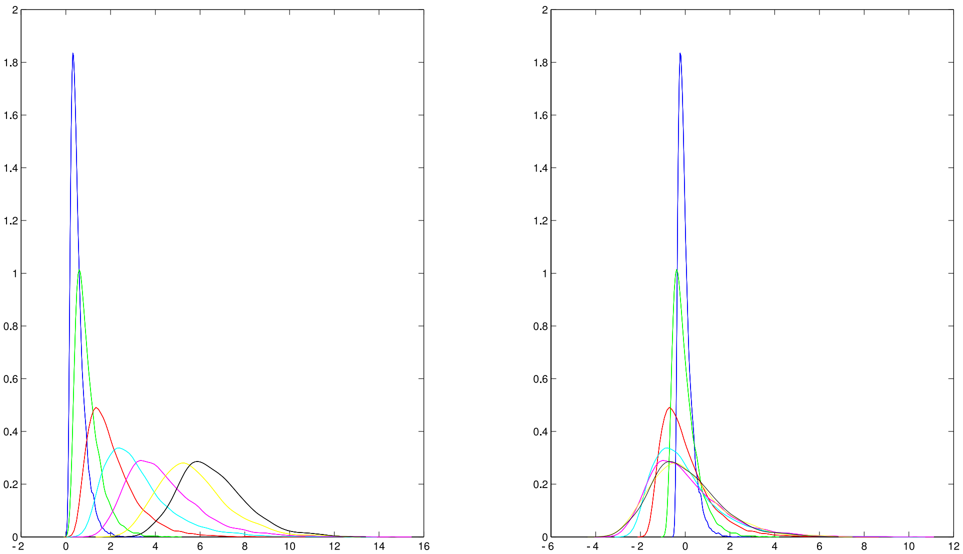

FIGURE 1.2. Left: Density of the length $T_{x\to B}$ for different values of ε (from left to right, $\varepsilon = 1, 0.5, 0.2, 0.1, 0.05, 0.02, 0.01$) when $V(x) = x^4/4 - x^2/2$, $A = -0.9$, $B = 0.9$, and $x = -0.89$. Right: Empirically centered versions of these densities.

where $\mathbb{E}_x$ denotes the expectation for the stochastic process starting from x. Let us also introduce the function u_s solution of

$$\begin{cases} A_\varepsilon u_s(x) = s u_s(x), \quad x \in (a,b), \\ u_s(a) = 0, \quad u_s(b) = 1. \end{cases} \tag{2.2}$$

It's formula ensures that $(u_s(X_t^{(\varepsilon)})e^{-st})_{t\geq 0}$ is a martingale and then

$$u_s(x) = \mathbb{E}_x\Big(u_s(X_H^{(\varepsilon)})e^{-sH}\Big) = \mathbb{E}_x\Big(e^{-sH}\mathbb{1}_{\{X_H^{(\varepsilon)}=b\}}\Big).$$

Consequently,

$$F_\varepsilon(s,x) = \frac{u_s(x)}{u_0(x)}. \tag{2.3}$$

This formula will play a crucial role in the following.

Remark 2.1. When $s = 0$, Equation (2.2) is easy to solve: for any $x \in (a,b)$,

$$u_0(x) = \mathbb{P}_x(T_b < T_a) = \frac{\int_a^x e^{V(s)/\varepsilon}\, ds}{\int_a^b e^{V(s)/\varepsilon}\, ds}. \tag{2.4}$$

2.2. *The h-transform of Doob.* The process $(X_t^{(\varepsilon)})_{t\geq 0}$ solution of the stochastic differential equation (1.1) conditionally to the event $\{T_b < T_a\}$ is still a Markov process. Moreover, it can be seen as the solution of a modified stochastic differential equation with a drift that depends on the exit probabilities for the process. This is the so-called *h-transform*.

Proposition 2.2. *Conditionally to the event $\{T_b < T_a\}$, the process $X^{(\varepsilon)}$ is a diffusion process and it is the solution of*

$$d\bar{X}_t^{(\varepsilon)} = \sqrt{2\varepsilon}\, dB_t + \left(-V'(\bar{X}_t^{(\varepsilon)}) + 2\varepsilon \frac{h'_\varepsilon(\bar{X}_t^{(\varepsilon)})}{h_\varepsilon(\bar{X}_t^{(\varepsilon)})} \mathbb{1}_{\{t<T_b\}} \right) dt \tag{2.5}$$

where, for any $x \in (a,b)$,

$$h_\varepsilon(x) = \frac{\int_a^x e^{V(s)/\varepsilon}\, ds}{\int_a^b e^{V(s)/\varepsilon}\, ds}.$$

See Day (1992) for the proof of this assertion *via* Girsanov's theorem. Similarly, one could write the equation satisfied by a diffusion process conditioned to reach a given point at a given time (see Marchand (2011) for instance). Notice that this construction can be generalized in a multidimensional context, but the the singular drift is not explicitly known in this case (see Lu and Nolen (2013)).

Remark 2.3. The additional drift is singular at point a and is equivalent to $2\varepsilon(x-a)^{-1}$ when $x \to a$. This ensures that Y cannot hit a in finite time (see Feller's condition in Revuz and Yor (1991)).

Let us associate to a potential V the modified drift induced by the h-transform on the interval (a,b):

$$b_V(x) = -V'(x) + 2\varepsilon \frac{h'_\varepsilon(x)}{h_\varepsilon(x)} = -V'(x) + 2\varepsilon \frac{e^{V(x)/\varepsilon}}{\int_a^x e^{V(s)/\varepsilon}\, ds}. \tag{2.6}$$

Lemma 2.4. *Let us assume that $x^* < a < 0 < b < y^*$ and that V satisfies Assumption 1.1. Then, for any $x \in (a,b)$,*

$$b_V(x) \xrightarrow[\varepsilon\to 0]{} |V'(x)|.$$

Proof: Since V is increasing on $(a,0)$ then, for any $x \in (a,0)$,

$$\int_a^x e^{V(s)/\varepsilon}\, ds \underset{\varepsilon\to 0}{\sim} \varepsilon \frac{e^{V(x)/\varepsilon}}{V'(x)} \quad \text{and} \quad b_V(x) \underset{\varepsilon\to 0}{\sim} V'(x) = |V'(x)|,$$

where, here and in the following, the notation $a(\varepsilon) \sim_{\varepsilon\to 0} b(\varepsilon)$ means that the ratio $a(\varepsilon)/b(\varepsilon)$ goes to 1 as $\varepsilon \to 0$. In other words, the h-transform turns the negative drift $-V'(x)$ to its opposite. Moreover, it is obvious that, for any $x > 0$, $h_\varepsilon(x)$ goes to 1 as $\varepsilon \to 0$ and $h'_\varepsilon(x)/h_\varepsilon(x)$ goes to 0 exponentially fast: in this case, $b_V(x) \to -V'(x) = |V'(x)|$. Finally, one can notice that

$$b_V(0) = \frac{2\varepsilon}{\int_a^0 e^{V(s)/\varepsilon}\, ds} \underset{\varepsilon\to 0}{\sim} \sqrt{\frac{8|V''(0)|\varepsilon}{\pi}},$$

since $V(s) \sim V''(0)s^2/2$ when s goes to zero. □

The h-transform and the previous lemma will be two major ingredients for the arguments below.

In the former proof, and in the following, we constantly use Laplace's method to get equivalents of integrals when ε tends to 0. Let us recall these classical results:

Lemma 2.5. *Let $[a,b)$ be some interval of $\mathbb{R}$ (with possibly $b=\infty$), $\psi : [a,b) \to \mathbb{R}$ a function continuous at point a such that $\psi(a) \neq 0$ and $\varphi : [a,b) \to \mathbb{R}$ a function of class $\mathcal{C}^2$ such that $\varphi' < 0$ on (a,b). Let us denote $f(\varepsilon) = \int_a^b \exp(\varphi(x)/\varepsilon)\, \psi(x)\, dx$. Then, we have:*

- *If $\varphi'(a)=0$ and $\varphi''(a)<0$,*

$$f(\varepsilon) \underset{\varepsilon\to 0}{\sim} \sqrt{\frac{\pi\varepsilon}{2|\varphi''(a)|}}\exp(\varphi(a)/\varepsilon)\,\psi(a).$$

- *If $\varphi'(a)<0$,*

$$f(\varepsilon) \underset{\varepsilon\to 0}{\sim} \frac{\varepsilon}{|\varphi'(a)|}\exp(\varphi(a)/\varepsilon)\,\psi(a).$$

3. Main example: the repulsive Ornstein-Uhlenbeck process

In this section, we deal with the simplest example of a potential that is smooth and strictly concave at the origin. We assume here that $V(x)=-\alpha x^2/2$ on the set $[-b,b]$ with $b,\alpha>0$, and then investigate the behavior of the process:

$$dY_t^{(\varepsilon,\alpha)} = \sqrt{2\varepsilon}dB_t + \alpha Y_t^{(\varepsilon,\alpha)}\,dt. \tag{3.1}$$

In the sequel, we denote

$$T_b^{\varepsilon,\alpha,x} = \inf\left\{t\geq 0\,:\,Y_t^{(\varepsilon,\alpha)}=b\right\} \quad \text{with } Y_0^{(\varepsilon,\alpha)}=x\in(-b,b).$$

For the sake of simplicity, we first deal with the case $\alpha=1$ and then we will get the general result thanks to a straightforward scaling. The strategy is to express the Laplace transform of this exit time in terms of special functions and then to derive its asymptotic form as ε goes to 0. In the sequel, T_b stands for $T_b^{(\varepsilon,1,x)}$.

Proposition 3.1. *Let $x\in(-b,b)$. For any $s>-1$, we have*

$$\mathbb{E}_x\left(e^{-sT_b}\,\middle|\,T_b<T_{-b}\right) \underset{\varepsilon\to 0}{\sim} \begin{cases} \Gamma(1+s)e^{-s(-\log\varepsilon+\log b+\log|x|)} & \text{if } x\in(-b,0),\\ \dfrac{2^{s/2}}{\sqrt{\pi}}\Gamma\left(\dfrac{1+s}{2}\right)e^{-s(-\log\sqrt{\varepsilon}+\log b)} & \text{if } x=0,\\ e^{-s(\log b-\log x)} & \text{if } x\in(0,b). \end{cases} \tag{3.2}$$

One can also notice that $\lim_{\varepsilon\to 0}\mathbb{E}_x\left(e^{-sT_b}\,\middle|\,T_b<T_{-b}\right)=\infty$ if $s\leq -1$.

Proof: The Laplace transform of the exit time is linked by (2.3) to the solution u_s of

$$\begin{cases} \varepsilon u_s''(x)+xu_s'(x)=su_s(x), & x\in(-b,b),\\ u_s(-b)=0,\\ u_s(b)=1. \end{cases} \tag{3.3}$$

Let us define $b_\varepsilon=b/\sqrt{\varepsilon}$ and the function v_s on $(-b_\varepsilon,b_\varepsilon)$ by $v_s(y)=u_s(y\sqrt{\varepsilon})$. Then v_s is the solution of

$$\begin{cases} v_s''(y)+yv_s'(y)=sv_s(y), & y\in(-b_\varepsilon,b_\varepsilon),\\ v_s(-b_\varepsilon)=0,\\ v_s(b_\varepsilon)=1. \end{cases} \tag{3.4}$$

As recalled in Section 2.1 (see (2.3)), one has

$$\mathbb{E}_x\left(e^{-sT_b}|T_b<T_{-b}\right)=\frac{u_s(x)}{u_0(x)}=\frac{v_s(x/\sqrt{\varepsilon})}{v_0(x/\sqrt{\varepsilon})}.$$

One can express the function v_s in terms of some special functions. Let $\nu > 0$ and define the parabolic cylinder function $D_{-\nu}$ as

$$D_{-\nu}(x) = \frac{1}{\Gamma(\nu)} e^{-x^2/4} \int_0^\infty t^{\nu-1} e^{-t^2/2 - xt}\, dt, \quad x \in \mathbb{R}.$$

The so-called Whittaker function $D_{-\nu}$ is solution of

$$D''_{-\nu}(x) - \left(\frac{x^2}{4} + \nu - \frac{1}{2}\right) D_{-\nu}(x) = 0.$$

See Abramowitz and Stegun (1964, ch.19) or Borodin and Salminen (2002, p.639) for further details. Define the function φ_ν by

$$\varphi_\nu(x) = e^{-x^2/4} D_{-\nu}(x).$$

A straightforward computation leads to

$$\varphi''_\nu(x) + x\varphi'_\nu(x) = (\nu - 1)\varphi_\nu(x). \tag{3.5}$$

In the sequel, s and ν are linked by the relation

$$\nu = s + 1 > 0.$$

Notice that $\psi_\nu\colon\ x \mapsto \varphi_\nu(-x)$ is also solution of (3.5), and that ψ_ν and φ_ν are linearly independent. Then, the solution of (3.4) is a linear combination of φ_ν and ψ_ν satisfying the boundary conditions. The function v_s is given by

$$v_s(x) = \frac{\varphi_\nu(-b_\varepsilon)\varphi_\nu(-x) - \varphi_\nu(b_\varepsilon)\varphi_\nu(x)}{\varphi_\nu(-b_\varepsilon)^2 - \varphi_\nu(b_\varepsilon)^2}. \tag{3.6}$$

Let us study the asymptotic behavior of $\varphi_\nu(b)$ and $\varphi_\nu(-b)$ as $b \to +\infty$. Laplace's method ensures that

$$\int_0^\infty t^{\nu-1} e^{-t^2/2} e^{-bt}\, dt \underset{b\to+\infty}{\sim} \frac{\Gamma(\nu)}{b^\nu}.$$

As a consequence,

$$\varphi_\nu(b) \underset{b\to+\infty}{\sim} \frac{e^{-b^2/2}}{b^\nu}.$$

Moreover,

$$\begin{aligned}\varphi_\nu(-b) &= \frac{1}{\Gamma(\nu)} \int_0^\infty t^{\nu-1} e^{-(t-b)^2/2}\, dt \\ &\underset{b\to+\infty}{\sim} \frac{\sqrt{2\pi}}{\Gamma(\nu)} b^{\nu-1}.\end{aligned}$$

In particular, one obtains that

$$\varphi_\nu(-b)^2 - \varphi_\nu(b)^2 \underset{b\to+\infty}{\sim} \varphi_\nu(-b)^2 \underset{b\to+\infty}{\sim} \frac{2\pi}{\Gamma(\nu)^2} b^{2(\nu-1)}.$$

Moreover, for any $\gamma \in (0,1)$, we get

$$\begin{aligned}\varphi_\nu(-b)\varphi_\nu(\gamma b) - \varphi_\nu(b)\varphi_\nu(-\gamma b) &\underset{b\to+\infty}{\sim} \frac{\sqrt{2\pi}}{\Gamma(\nu)} b^{\nu-1} \frac{e^{-\gamma^2 b^2/2}}{(\gamma b)^\nu} - \frac{\sqrt{2\pi}}{\Gamma(\nu)} (\gamma b)^{\nu-1} \frac{e^{-b^2/2}}{b^\nu} \\ &\underset{b\to+\infty}{\sim} \frac{\sqrt{2\pi}}{\Gamma(\nu)} \frac{e^{-\gamma^2 b^2/2}}{\gamma^\nu b}.\end{aligned}$$

As a conclusion

$$\frac{\varphi_\nu(-b)\varphi_\nu(\gamma b)-\varphi_\nu(b)\varphi_\nu(-\gamma b)}{\varphi_\nu(-b)^2-\varphi_\nu(b)^2} \underset{b\to+\infty}{\sim} \frac{\Gamma(\nu)}{\sqrt{2\pi}}\frac{e^{-\gamma^2b^2/2}}{\gamma^\nu b^{2\nu-1}} = \frac{\Gamma(\nu)}{\sqrt{2\pi}}\frac{e^{-\gamma^2b^2/2}}{(\gamma b)^\nu b^{\nu-1}}. \tag{3.7}$$

One can then deduce the asymptotic behavior of v_s solution of Equation (3.4) at the point $x/\sqrt{\varepsilon}$ (with $x<0$) replacing in Equation (3.7) b by $b_\varepsilon = b/\sqrt{\varepsilon}$ and γ by $-x/b$ with $\gamma \in (0,1)$. Since $\nu = s+1$, this leads to

$$v_s(x/\sqrt{\varepsilon}) \underset{\varepsilon\to 0}{\sim} \frac{\Gamma(1+s)}{\sqrt{2\pi}}\frac{e^{-x^2/(2\varepsilon)}}{(-x/\sqrt{\varepsilon})^{s+1}(b/\sqrt{\varepsilon})^s},$$

and

$$\frac{v_s(x/\sqrt{\varepsilon})}{v_0(x/\sqrt{\varepsilon})} \underset{\varepsilon\to 0}{\sim} \frac{\Gamma(1+s)}{(-x/\sqrt{\varepsilon})^s(b/\sqrt{\varepsilon})^s} = \Gamma(1+s)\left(\frac{\varepsilon}{|x|b}\right)^s.$$

This is the expression of the Laplace transform in Equation (3.2) when $x \in (-b,0)$. The two other cases are easier to deal with. If $x=0$, since $v_0(0)=1/2$, one has

$$\frac{v_s(0)}{v_0(0)} \underset{\varepsilon\to 0}{\sim} \frac{2\varphi_\nu(0)}{\varphi_\nu(-b_\varepsilon)} \underset{\varepsilon\to 0}{\sim} \sqrt{\frac{2}{\pi}}\frac{1}{b_\varepsilon^s}\int_0^{+\infty} t^s e^{-t^2/2}\,dt = \frac{2^{s/2}}{\sqrt{\pi}}\Gamma\left(\frac{1+s}{2}\right)\frac{1}{b_\varepsilon^s}.$$

At last, if $x=\gamma b$ with $\gamma\in(0,1)$, then

$$\frac{v_s(\gamma b_\varepsilon)}{v_0(\gamma b_\varepsilon)} \underset{\varepsilon\to 0}{\sim} \frac{\varphi_\nu(-\gamma b_\varepsilon)}{\varphi_\nu(-b_\varepsilon)} = \gamma^s = \left(\frac{x}{b}\right)^s.$$

□

Remark 3.2. The parabolic cylinder functions $D_{-\nu}$ also appear in Breiman (1967, Section 2), where the author studies the first exit time from a square root boundary for the Brownian motion.

Proposition 3.1 yields the following convergence in distribution.

Theorem 3.3. *Let $\alpha>0$ and $x\in(-b,b)$. We have, conditionally to the event $\left\{T_b^{(\varepsilon,\alpha,x)} < T_{-b}^{(\varepsilon,\alpha,x)}\right\}$,*

- *if $x\in(-b,0)$*

$$T_b^{(\varepsilon,\alpha,x)} + \frac{1}{\alpha}\log\varepsilon \xrightarrow[\varepsilon\to 0]{\mathcal{L}} \frac{1}{\alpha}(\log(|x|b)+G-\log\alpha),$$

- *if $x=0$*

$$T_b^{(\varepsilon,\alpha,x)} + \frac{1}{\alpha}\log\sqrt{\varepsilon} \xrightarrow[\varepsilon\to 0]{\mathcal{L}} \frac{1}{\alpha}\left(\log b+\tilde{G}-\log\sqrt{\alpha}\right),$$

- *if $x\in(0,b)$*

$$T_b^{(\varepsilon,\alpha,x)} \xrightarrow[\varepsilon\to 0]{\mathcal{L}} \frac{1}{\alpha}(\log b-\log x),$$

where the law of G is the standard Gumbel distribution and $\tilde{G}$ is a random variable with Laplace transform given by

$$\mathbb{E}\left(e^{-s\tilde{G}}\right) = \begin{cases} \dfrac{2^{s/2}}{\sqrt{\pi}}\Gamma\left(\dfrac{1+s}{2}\right) & \text{if } s>-1,\\ +\infty & \text{otherwise.}\end{cases}$$

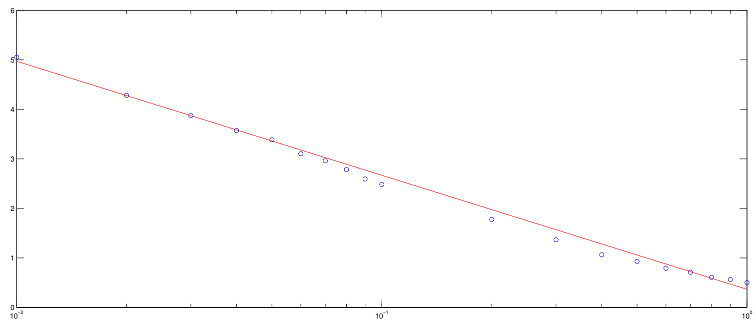

FIGURE 3.3. Mean length of the reactive path for the repulsive Ornstein-Uhlenbeck process $dY_t^{(\varepsilon)} = \sqrt{2\varepsilon}dB_t + Y_t^{(\varepsilon)}\,dt$, with $Y_0^{(\varepsilon)} = -0.89$, on the set $[-0.9, 0.9]$ as a function of $\log\varepsilon$ (see Theorem 3.3). The 95% confidence intervals are of the size of the points. The function $\log\varepsilon \mapsto -\log\varepsilon + \log(|-0.89| \times 0.9) + \gamma$ is drawn in red. These results have been obtained with the algorithm described in Cérou et al. (2011).

Proof: The case $\alpha = 1$ is a straightforward consequence of Proposition 3.1. Moreover, for any positive constants τ and σ, and for any $t \geq 0$, one has

$$\begin{aligned}\sigma Y_{\tau t}^{(\varepsilon,\alpha)} &= \sigma Y_0^{(\varepsilon,\alpha)} + \sigma\sqrt{2\varepsilon}B_{\tau t} + \sigma\alpha\int_0^{\tau t} Y_s^{(\varepsilon,\alpha)}\,ds \\ &\overset{\mathcal{L}}{=} \sigma Y_0^{(\varepsilon,\alpha)} + \sqrt{\tau\sigma^2}\sqrt{2\varepsilon}B_t + \alpha\tau\int_0^t \sigma Y_{\tau u}^{(\varepsilon,\alpha)}\,du.\end{aligned}$$

This ensures that if $\sigma = \sqrt{\alpha}$ and $\tau = 1/\alpha$, then the process $(\sigma Y_{\tau t}^{(\varepsilon,\alpha)})_{t\geq 0}$ is solution of Equation (3.1) with $\alpha = 1$ and the initial condition $\sigma Y_0^{(\varepsilon,\alpha)}$. In particular,

$$\mathcal{L}\Big(T_b^{(\varepsilon,\alpha,x)} \,|\, T_b^{(\varepsilon,\alpha,x)} < T_{-b}^{(\varepsilon,\alpha,x)}\Big) = \mathcal{L}\Big(\alpha^{-1} T_{b/\sqrt{\alpha}}^{(\varepsilon,1,x/\sqrt{\alpha})} \,|\, T_{b/\sqrt{\alpha}}^{(\varepsilon,1,x/\sqrt{\alpha})} < T_{-b/\sqrt{\alpha}}^{(\varepsilon,1,x/\sqrt{\alpha})}\Big).$$

The result for $\alpha \neq 1$ is a straightforward consequence of the result for $\alpha = 1$. $\square$

Notice that the formulas in Theorem 3.3 admit a limit when x goes to $-b$. Before coming back to the general case, let us conclude this section with a few remarks about the case of the Ornstein-Uhlenbeck process.

Remark 3.4. Let us discuss the asymptotic behavior of the formulas in Theorem 3.3 for the length of the reactive path when $x \in (-b, 0)$ and ε goes to 0, assuming for simplicity that $\alpha = 1$. The time $\log(b/\sqrt{\varepsilon})$ is the time needed by the deterministic process $Y^{(0,1)}$ to go from $\sqrt{\varepsilon}$ to b since $Y_t^{(0,1)} = e^t\sqrt{\varepsilon}$. The Freidlin-Wentzell theory tells us that the first part of the reactive path (from x to $-\sqrt{\varepsilon}$) has a similar length $\log(|x|/\sqrt{\varepsilon})$. Finally, the Gumbel variable G accounts for the (asymptotic) random time needed by $Y^{(\varepsilon,1)}$ to go from $-\sqrt{\varepsilon}$ to $\sqrt{\varepsilon}$.

Remark 3.5. It is easy to check from the proof that the results of Proposition 3.1 are still valid if $b = b_\varepsilon$ and $x = x_\varepsilon$ depend on ε as long as $b_\varepsilon/\sqrt{\varepsilon}$ and $x_\varepsilon/\sqrt{\varepsilon}$ go to infinity when ε goes to zero. For example, if $b_\varepsilon > 0$ is such that $\lim_{\varepsilon\to 0} b_\varepsilon/\sqrt{\varepsilon} = \infty$ and $x_\varepsilon \in (-b_\varepsilon, 0)$ is such that $\lim_{\varepsilon\to 0} x_\varepsilon/\sqrt{\varepsilon} = -\infty$, then

$$T_{b_\varepsilon}^{(\varepsilon,\alpha,x_\varepsilon)} + \frac{1}{\alpha}\left(\log\varepsilon - \log(|x_\varepsilon|b_\varepsilon)\right) \xrightarrow[\varepsilon\to 0]{\mathcal{L}} \frac{1}{\alpha}\left(G - \log\alpha\right).$$

This remark will be useful in Section 4.3.

Remark 3.6. Figure 3.3 illustrates Theorem 3.3 for the so-called repulsive Ornstein-Uhlenbeck process $dY_t^{(\varepsilon)} = \sqrt{2\varepsilon}dB_t + Y_t^{(\varepsilon)}\,dt$, with $Y_0^{(\varepsilon)} = -0.89$, on the set $[-0.9, 0.9]$. Denoting $T_{-0.89\to 0.9}$ the length of the reactive path from -0.89 to 0.9, then Theorem 3.3 ensures that $\mathbb{E}[T_{-0.89\to 0.9}]$ is equivalent to $-\log\varepsilon + \log(|-0.89| \times 0.9) + \gamma$, when ε goes to zero (γ stands here for Euler's constant). Figure 3.3 compares this theoretical result with the empirical means obtained thanks to the algorithm described in Cérou et al. (2011) for ε ranging from 0.01 to 1.

4. The general (strictly convex) case

Let us now come back to the general strictly convex case described in Section 1. We recall the notations (see Figure 1.1). The potential V has exactly two local minima $x^* < 0$ and $y^* > 0$ and a local maximum $z^* = 0$. Moreover, V' is positive on $(x^*, 0)$ and negative on $(0, y^*)$ and

$$V(0) = 0, \quad V'(0) = 0, \quad \text{and} \quad V''(0) = -\alpha < 0.$$

Let us consider $A \in (x^*, 0)$, $B \in (0, y^*)$ and $x \in (A, 0)$. We are interested in the behavior of

$$T_{x\to B} = \inf\left\{t > 0 \,:\, X_t^{(\varepsilon)} = B\right\} \quad \text{cond. to the event } \left\{X_0^{(\varepsilon)} = x,\ T_B < T_A\right\},$$

when ε goes to zero.

According to the Markov property, and considering the initial point $x \in (A, 0)$, the strategy is to decompose the reactive path from x to B into three independent pieces:

$$H = T_{x\to -c_\varepsilon} + T_{-c_\varepsilon\to b_\varepsilon} + T_{b_\varepsilon\to B} \tag{4.1}$$

on the event $\{T_B < T_A\}$ where $0 < c_\varepsilon < b_\varepsilon < |x| \wedge B$ will be specified in the sequel. More precisely, we will choose

$$b_\varepsilon = \varepsilon^\beta \quad \text{and} \quad c_\varepsilon = \varepsilon^\gamma \quad \text{with} \quad \frac{2}{5} < \beta < \gamma < \frac{1}{2}.$$

The first and third times in (4.1) are essentially deterministic, as specified by the following result.

Proposition 4.1. *If $0 < \beta, \gamma < 1/2$, then, conditionally to the event $\{T_B < T_A\}$,*

$$T_{b_\varepsilon\to B} - t_{b_\varepsilon\to B} \xrightarrow[\varepsilon\to 0]{\mathbb{P}} 0 \quad \textit{and} \quad T_{x\to -c_\varepsilon} - t_{-c_\varepsilon\to x} \xrightarrow[\varepsilon\to 0]{\mathbb{P}} 0,$$

where $t_{b_\varepsilon\to B}$ is the time for the unnoised process to reach B from $b_\varepsilon \in (0, B)$:

$$t_{b_\varepsilon\to B} = -\int_{b_\varepsilon}^{B} \frac{1}{V'(s)}\,ds,$$

and $t_{-c_\varepsilon\to x}$ is the time for the unnoised process to reach x from $-c_\varepsilon \in (x, 0)$:

$$t_{-c_\varepsilon\to x} = -\int_{-c_\varepsilon}^{x} \frac{1}{V'(s)}\,ds.$$

This is proved in Sections 4.1 and 4.2. In Section 4.3 we compare the second time in (4.1) to the reactive time of an Ornstein-Uhlenbeck process.

4.1. *Going down is easy.* The easiest part is to study the third time $T_{b_\varepsilon \to B}$. Our goal here is to prove that, starting at b_ε, the process $X^{(\varepsilon)}$ is close to the deterministic path $(x_t)_{t\geq 0}$ solution of the ordinary differential equation

$$\begin{cases} \dot{x}_t = -V'(x_t) & t \geq 0, \\ x_0 = b_\varepsilon. \end{cases}$$

In this aim, we need to state a few intermediate results. First, it is readily seen that, starting at b_ε, the probability for the process $(X_t^{(\varepsilon)})_{t\geq 0}$ to hit 0 before B goes to 0 at an exponential rate when ε goes to 0. Indeed, we have (see Equation (2.4)):

$$\mathbb{P}_{b_\varepsilon}(T_0 < T_B) = \frac{\int_{b_\varepsilon}^B e^{V(s)/\varepsilon} ds}{\int_0^B e^{V(s)/\varepsilon} ds} \leq \frac{B e^{V(b_\varepsilon)/\varepsilon}}{\int_0^B e^{V(s)/\varepsilon} ds}.$$

Using the fact that $\int_0^B e^{V(s)/\varepsilon} ds \underset{\varepsilon\to 0}{\sim} \sqrt{\frac{\pi\varepsilon}{2\alpha}}$, $b_\varepsilon = \varepsilon^\beta$ with $\beta < 1/2$ and (1.5), we thus easily get that $\mathbb{P}_{b_\varepsilon}(T_0 < T_B)$ converges exponentially fast to 0 as ε goes to 0. In the following, we will denote Ω_ε the event on which this does not occur, so that $\mathbb{P}(\Omega_\varepsilon)$ goes to 1 when ε goes to 0.

Of course, this will also be true for the event Ω_x which is defined as: the process starts at a fixed point $x \in (0, B)$ (independent of ε) and does not hit 0 before B. Again, $\mathbb{P}(\Omega_x)$ goes to 1 when ε goes to 0. Then, starting at $x \in (0, B)$, our aim is to compare the deterministic path $(x_t)_{t\geq 0}$ solution of the ordinary differential equation

$$\begin{cases} \dot{x}_t = -V'(x_t) & t \geq 0, \\ x_0 = x, \end{cases} \tag{4.2}$$

and the random process

$$\begin{cases} dX_t^{(\varepsilon)} = -V'(X_t^{(\varepsilon)})\, dt + \sqrt{2\varepsilon} dB_t & t \geq 0, \\ X_0^{(\varepsilon)} = x. \end{cases}$$

For this, let us introduce $c \in (B, y^*)$ such that $c - B < B - x$, the deterministic time $t_c = t_{x\to c} = \inf\{t > 0 \ : \ x_t = c\}$ and the stochastic time

$$T_c = T_{x\to c} = \inf\left\{t > 0 \ : \ X_t^{(\varepsilon)} = c\right\}.$$

Lemma 4.2. *Define* $K := \sup_{s\in[0,c]} |V''(s)|$, *then*

$$\mathbb{P}\left(\Omega_x \cap \left\{\sup_{0\leq s\leq t_c\wedge T_c} |X_s^{(\varepsilon)} - x_s| \geq \eta\right\}\right) \leq 2\exp\left(-\frac{\eta^2 e^{-2Kt_c}}{4\varepsilon t_c}\right).$$

Proof: Let us assume that we work on the event Ω_x. For any $t \leq t_c \wedge T_c$,

$$X_t^{(\varepsilon)} - x_t = -\int_0^t (V'(X_s^{(\varepsilon)}) - V'(x_s))\, ds + \sqrt{2\varepsilon} B_t.$$

The Gronwall Lemma ensures that

$$\sup_{0\leq s\leq t_c\wedge T_c} |X_s^{(\varepsilon)} - x_s| \leq \sqrt{2\varepsilon} e^{K(t_c\wedge T_c)} \sup_{0\leq s\leq t_c\wedge T_c} |B_s| \leq \sqrt{2\varepsilon} e^{Kt_c} \sup_{0\leq s\leq t_c} |B_s|.$$

Finally, the reflection principle for the Brownian motion ensures that $\sup_{0\le s\le t} B_s$ has the law of $|B_t|$. As a consequence, for any $r, t \ge 0$,

$$\mathbb{P}\left(\sup_{0\le s\le t}|B_s| \ge r\right) \le 2\mathbb{P}\left(\sup_{0\le s\le t} B_s \ge r\right) = 2\mathbb{P}(|B_t| \ge r) \le 2e^{-r^2/(2t)}.$$

This concludes the proof. □

The first consequence of this result is that the stochastic time $T_{x\to B}$ required by the random process to go from $x \in (0,B)$ to B converges to the deterministic time $t_{x\to B}$ as $\varepsilon \to 0$.

Corollary 4.3. *Let* $0 < x < B$*, then*

$$T_{x\to B} \xrightarrow[\varepsilon\to 0]{\mathbb{P}} t_{x\to B}.$$

Proof: Since we will apply the result of the previous lemma, we still work on the event Ω_x. Let us denote η a real number such that $0 < \eta < c - B$. Then, on the event $\Omega_x \cap \left\{\sup_{0\le s\le t_c\wedge T_c}|X_s^{(\varepsilon)} - x_s| \le \eta\right\}$, the random time $T_{x\to B}$ belongs to the deterministic interval $[t_{x\to B-\eta}, t_{x\to B+\eta}]$. In other words,

$$\int_{B-\eta}^{B}\frac{ds}{V'(s)} = -t_{B-\eta\to B} \le T_{x\to B} - t_{x\to B} \le t_{B\to B+\eta} = -\int_{B}^{B+\eta}\frac{ds}{V'(s)}.$$

As a consequence, for any $\eta \in (0, c-B)$,

$$|T_{x\to B} - t_{x\to B}| \le \eta \times \sup_{s\in[B-\eta,B+\eta]}\frac{1}{|V'(s)|}.$$

Finally, for any $\eta \in (0, c-B)$,

$$\mathbb{P}\left(\Omega_x \cap \left\{|T_{x\to B} - t_{x\to B}| \ge \eta \times \sup_{s\in[B-\eta,B+\eta]}\frac{1}{|V'(s)|}\right\}\right) \le 2\exp\left(-\frac{\eta^2 e^{-2Kt_c}}{4\varepsilon t_c}\right),$$

where $t_c = t_{x\to c}$. This concludes the proof of the corollary. □

Our next goal is to prove that this result still holds if the starting point, namely $b_\varepsilon = \varepsilon^\beta$, goes to 0 sufficiently slowly as $\varepsilon \to 0$, that means if $\beta < 1/2$. Let us fix $D \in (b_\varepsilon, B)$ (for sufficiently small ε) such that

$$\sup_{s\in[0,D]}|V''(s)| < \frac{\alpha}{2\beta}.$$

This is always possible since $\beta < 1/2$, $|V''(0)| = \alpha$, and V is assumed to be smooth. Then, as previously, we fix $c \in (D, B)$ such that $c - D < D - b_\varepsilon$, and

$$K := \sup_{s\in[0,c]}|V''(s)| < \frac{\alpha}{2\beta}.$$

Corollary 4.4. *If* $0 < b_\varepsilon = \varepsilon^\beta$ *with* $\beta < 1/2$*, then*

$$|T_{b_\varepsilon\to D} - t_{b_\varepsilon\to D}| \xrightarrow[\varepsilon\to 0]{\mathbb{P}} 0.$$

Proof: Here, we work on the event Ω_ε, which is not a problem since, as mentioned above, $\mathbb{P}(\Omega_\varepsilon)$ goes to 1 as ε goes to zero. The first part of the proof is similar to the ones of Lemma 4.2 and Corollary 4.3. For any $\eta \in (0, c - D)$,

$$\mathbb{P}\left(\Omega_\varepsilon \cap \left\{|T_{b_\varepsilon\to D} - t_{b_\varepsilon\to D}| \geq \eta \times \sup_{s\in[D-\eta,D+\eta]} \frac{1}{|V'(s)|}\right\}\right) \leq 2\exp\left(-\frac{\eta^2 e^{-2Kt_c}}{4\varepsilon t_c}\right),$$

where $t_c = t_{b_\varepsilon\to c}$. Moreover, since $V'(s) \sim_{s\to 0} -\alpha s$, we have

$$t_{b_\varepsilon\to c} = -\int_{b_\varepsilon}^{c} \frac{ds}{V'(s)} = -\frac{1}{\alpha}\log b_\varepsilon + O_\varepsilon(1).$$

As a consequence,

$$\frac{e^{-2Kt_c}}{4\varepsilon t_c} \underset{\varepsilon\to 0}{\sim} \frac{\alpha\varepsilon^{\frac{2K\beta}{\alpha}-1}}{-4\beta\log\varepsilon} \xrightarrow[\varepsilon\to 0]{} +\infty.$$

This proves the convergence in probability of $T_{b_\varepsilon\to D}$ as ε goes to 0. □

Finally, according to the Markov property, we can summary the previous results by decomposing the path from b_ε to B into two independent pieces:

$$T_{b_\varepsilon\to B} = T_{b_\varepsilon\to D} + T_{D\to B}.$$

Using Corollaries 4.3 and 4.4, we immediately get the following proposition.

Proposition 4.5. *If* $0 < b_\varepsilon = \varepsilon^\beta$ *with* $\beta < 1/2$*, then*

$$|T_{b_\varepsilon\to B} - t_{b_\varepsilon\to B}| \xrightarrow[\varepsilon\to 0]{\mathbb{P}} 0 \quad \textit{where} \quad t_{b_\varepsilon\to B} = -\int_{b_\varepsilon}^{B} \frac{ds}{V'(s)}.$$

Remark 4.6. If V is given by (1.6), one can compute the expression of the solution $(x_t)_{t\geq 0}$ of (4.2). Let us define the function Ψ on $(0,1)$ by

$$\Psi(x) = \log\left(\frac{x}{\sqrt{1-x^2}}\right).$$

Notice that

$$\Psi'(x) = \frac{1}{x} - \frac{1/2}{x-1} - \frac{1/2}{x+1} = -\frac{1}{V'(x)}.$$

As a consequence, the derivative of $t \mapsto \Psi(x_t)$ is equal to 1 and

$$x_t = \Psi^{-1}(\Psi(x) + t).$$

Moreover, the elapsed time from $x \in (0, B)$ to $B \in (0,1)$ is given by

$$t_{x\to B} = \Psi(B) - \Psi(x) = -\log(x) + \Psi(B) + \frac{1}{2}\log(1-x^2).$$

As was just proved, this result still holds when $x = b_\varepsilon$ as long as $0 < \beta < 1/2$.

4.2. *The climbing period.*

Proposition 4.7. *If* $c_\varepsilon = \varepsilon^\gamma$ *with* $\gamma < 1/2$*, then, for* $x \in (A, 0)$*, conditionally to the event* $\{T_{-c_\varepsilon} < T_A\}$*,*

$$|T_{x\to -c_\varepsilon} - t_{-c_\varepsilon\to x}| \xrightarrow[\varepsilon\to 0]{\mathbb{P}} 0 \quad \textit{where} \quad t_{-c_\varepsilon\to x} = -\int_{-c_\varepsilon}^{x} \frac{ds}{V'(s)}.$$

Proof: One has to consider the h-transformed process and use the fact that the new drift converges to $V'(s)$ uniformly on $[A + \delta, -c_\varepsilon]$ for any δ small enough as ε goes to 0, see Lemma 2.4 above. □

4.3. *Central behavior.* Let us finally study the behavior of $T_{-c_\varepsilon \to b_\varepsilon}$ conditionally to the event $\{T_{b_\varepsilon} < T_A\}$. In all what follows, $b_\varepsilon = \varepsilon^\beta$, $c_\varepsilon = \varepsilon^\gamma$, with $0 < \beta < \gamma < 1/2$. Additional conditions on β will be made precise below.

The sketch of proof is as follows:

(1) Prove that one may assume that the process does not go below $-b_\varepsilon$;
(2) Rescale space to map $(-b_\varepsilon, b_\varepsilon)$ onto $(-1,1)$;
(3) Consider the h-transformed process to get the evolution of the process conditioned on $\{T_1 < T_{-1}\}$;
(4) Introduce the h-transformed repulsive Ornstein-Uhlenbeck process;
(5) Compare the drifts;
(6) Use Theorem 4.3 in Day (1992);
(7) Conclude.

Step 1. The first step is to notice that it is equivalent to look at $T_{-c_\varepsilon \to b_\varepsilon}$ conditionally to $\{T_{b_\varepsilon} < T_{-b_\varepsilon}\}$ or conditionally to $\{T_{b_\varepsilon} < T_A\}$.

Lemma 4.8. *If* $0 < \beta < \gamma < 1/2$*, there exists a constant* $C > 0$ *such that, for any* $s > 0$

$$1 - C\varepsilon^{\gamma-\beta} \le \frac{\mathbb{E}_{-c_\varepsilon}\left(e^{-sH_{A,b_\varepsilon}} | T_{b_\varepsilon} < T_A\right)}{\mathbb{E}_{-c_\varepsilon}(e^{-sH_{-b_\varepsilon,b_\varepsilon}} | T_{b_\varepsilon} < T_{-b_\varepsilon})} \le 1 + C\varepsilon^{\gamma-\beta}.$$

Proof: By continuity,

$$\{T_{b_\varepsilon} < T_A\} = \{T_{b_\varepsilon} < T_{-b_\varepsilon}\} \cup \{T_{-b_\varepsilon} < T_{b_\varepsilon} < T_A\},$$

where the two sets on the right hand side are disjoints. Moreover, the strong Markov property ensures that, for any $s \ge 0$,

$$\begin{aligned} 0 &\le \mathbb{E}_{-c_\varepsilon}\left(e^{-sH_{A,b_\varepsilon}} \mathbb{1}_{\{T_{-b_\varepsilon} < T_{b_\varepsilon} < T_A\}}\right) \\ &\le \mathbb{E}_{-b_\varepsilon}\left(e^{-sH_{A,b_\varepsilon}} \mathbb{1}_{\{T_{b_\varepsilon} < T_A\}}\right) \\ &\le \mathbb{P}_{-b_\varepsilon}(T_{-c_\varepsilon} < T_A)\mathbb{E}_{-c_\varepsilon}\left(e^{-sH_{A,b_\varepsilon}} \mathbb{1}_{\{T_{b_\varepsilon} < T_A\}}\right). \end{aligned}$$

As a consequence, for any $s \ge 0$,

$$1 \le \frac{\mathbb{E}_{-c_\varepsilon}\left[e^{-sH_{A,b_\varepsilon}} \mathbb{1}_{\left\{T_{b_\varepsilon} < T_A\right\}}\right]}{\mathbb{E}_{-c_\varepsilon}\left[e^{-sH_{-b_\varepsilon,b_\varepsilon}} \mathbb{1}_{\left\{T_{b_\varepsilon} < T_{-b_\varepsilon}\right\}}\right]} \le 1 + \mathbb{P}_{-b_\varepsilon}(T_{-c_\varepsilon} < T_A) \le \frac{1}{1 - \mathbb{P}_{-b_\varepsilon}(T_{-c_\varepsilon} < T_A)}.$$

Taking $s = 0$ in this equation leads to

$$1 - \mathbb{P}_{-b_\varepsilon}(T_{-c_\varepsilon} < T_A) \le \frac{\mathbb{P}_{-c_\varepsilon}(T_{b_\varepsilon} < T_{-b_\varepsilon})}{\mathbb{P}_{-c_\varepsilon}(T_{b_\varepsilon} < T_A)} \le 1.$$

Consequently,

$$1 - \mathbb{P}_{-b_\varepsilon}(T_{-c_\varepsilon} < T_A) \le \frac{\mathbb{E}_{-c_\varepsilon}\left(e^{-sH_{A,b_\varepsilon}} | T_{b_\varepsilon} < T_A\right)}{\mathbb{E}_{-c_\varepsilon}(e^{-sH_{-b_\varepsilon,b_\varepsilon}} | T_{b_\varepsilon} < T_{-b_\varepsilon})} \le 1 + \mathbb{P}_{-b_\varepsilon}(T_{-c_\varepsilon} < T_A).$$

To conclude, one just has to remark that, since $V(-b_\varepsilon) \le V(-c_\varepsilon)$,

$$\mathbb{P}_{-b_\varepsilon}(T_{-c_\varepsilon} < T_A) = \frac{\int_A^{-b_\varepsilon} e^{V(s)/\varepsilon}\, ds}{\int_A^{-c_\varepsilon} e^{V(s)/\varepsilon}\, ds} \underset{\varepsilon \to 0}{\sim} \varepsilon^{\gamma-\beta} e^{(V(-b_\varepsilon) - V(-c_\varepsilon))/\varepsilon} \le \varepsilon^{\gamma-\beta}.$$

$\square$

Step 2. Let us define $\eta_\varepsilon = \varepsilon/b_\varepsilon^2$ and the process Y by $Y_t = X_t^{(\varepsilon)}/b_\varepsilon$ (dropping for simplicity the explicit dependence on ε in the notation for Y). Obviously, if $X_0^{(\varepsilon)}$ is equal to $-c_\varepsilon$, then Y is solution of

$$\begin{cases} dY_t = \sqrt{2\eta_\varepsilon} dB_t - \dfrac{V'(b_\varepsilon Y_t)}{b_\varepsilon}\, dt, \\ Y_0 = -c_\varepsilon/b_\varepsilon. \end{cases}$$

In terms of Y, we are interested in the hitting time of 1 conditionally to the event $\{T_1 < T_{-1}\}$.

Step 3. Thanks to the h-transform of Doob, one can see Y, conditionally to the event $\{T_1 < T_{-1}\}$, as a diffusion process. Define, for any $y \in (-1,1)$,

$$h_\varepsilon(y) = \frac{\int_{-1}^{y} e^{V(b_\varepsilon s)/\varepsilon}\, ds}{\int_{-1}^{1} e^{V(b_\varepsilon s)/\varepsilon}\, ds} \quad \text{and} \quad \frac{h_\varepsilon'(y)}{h_\varepsilon(y)} = \frac{e^{V(b_\varepsilon y)/\varepsilon}}{\int_{-1}^{y} e^{V(b_\varepsilon s)/\varepsilon}\, ds}.$$

Conditionally to $\{T_1 < T_{-1}\}$, the process Y is solution of

$$\begin{cases} dY_t = \sqrt{2\eta_\varepsilon} dB_t + \left(-\dfrac{V'(b_\varepsilon Y_t)}{b_\varepsilon} + 2\eta_\varepsilon \dfrac{h_\varepsilon'(Y_t)}{h_\varepsilon(Y_t)} \mathbb{1}_{\{t \le T_1\}} \right) dt, \\ Y_0 = -c_\varepsilon/b_\varepsilon. \end{cases}$$

Step 4. Similarly, the repulsive Ornstein-Uhlenbeck process $(Z_t)_{t\ge 0}$ solution of

$$\begin{cases} dZ_t = \sqrt{2\eta_\varepsilon}\, dB_t + \alpha Z_t\, dt, \\ Z_0 = -c_\varepsilon/b_\varepsilon, \end{cases}$$

evolves, conditionally to the event $\{T_1 < T_{-1}\}$, as

$$\begin{cases} dZ_t = \sqrt{2\eta_\varepsilon} dB_t + \left(\alpha Z_t + 2\eta_\varepsilon \dfrac{g_\varepsilon'(Z_t)}{g_\varepsilon(Z_t)} \mathbb{1}_{\{t \le T_1\}} \right) dt, \\ Z_0 = -c_\varepsilon/b_\varepsilon, \end{cases}$$

where

$$g_\varepsilon(y) = \frac{\int_{-1}^{y} e^{-\alpha s^2/(2\eta_\varepsilon)}\, ds}{\int_{-1}^{1} e^{-\alpha s^2/(2\eta_\varepsilon)}\, ds} \quad \text{and} \quad \frac{g_\varepsilon'(y)}{g_\varepsilon(y)} = \frac{e^{-\alpha y^2/(2\eta_\varepsilon)}}{\int_{-1}^{y} e^{-\alpha s^2/(2\eta_\varepsilon)}\, ds}.$$

Step 5. Let us now notice that the drifts of the stochastic differential equations that drive Y and Z conditionally to the event $\{T_1 < T_{-1}\}$ are close.

Lemma 4.9. *Under Assumption 1.1, if* $4/9 < \beta < 1/2$*, then*

$$\frac{1}{\eta_\varepsilon} \times \sup_{y \in (-1,-1]} \left| \left(-\frac{V'(b_\varepsilon y)}{b_\varepsilon} + 2\eta_\varepsilon \frac{h_\varepsilon'(y)}{h_\varepsilon(y)} \right) - \left(\alpha y + 2\eta_\varepsilon \frac{g_\varepsilon'(y)}{g_\varepsilon(y)} \right) \right| \xrightarrow[\varepsilon \to 0]{} 0. \tag{4.3}$$

Proof of Lemma 4.9: Thanks to Assumption 1.1, as soon as $b_\varepsilon < \delta$, we have, for any $y \in [-1,1]$,

$$\left| -\frac{V'(b_\varepsilon y)}{b_\varepsilon} - \alpha y \right| \le K b_\varepsilon y^2 \le K b_\varepsilon,$$

so that

$$\frac{1}{\eta_\varepsilon} \times \sup_{y \in (-1,-1]} \left| -\frac{V'(b_\varepsilon y)}{b_\varepsilon} - \alpha y \right| \xrightarrow[\varepsilon \to 0]{} 0$$

as soon as $\beta > 1/3$. It remains to prove that $\sup_{y\in(-1,-1]} |\Delta_\varepsilon(y)|$ goes to zero when ε goes to zero, where

$$\Delta_\varepsilon(y) := \frac{h_\varepsilon'(y)}{h_\varepsilon(y)} - \frac{g_\varepsilon'(y)}{g_\varepsilon(y)} = \frac{e^{V(b_\varepsilon y)/\varepsilon}}{\int_{-1}^{y} e^{V(b_\varepsilon s)/\varepsilon}\, ds} - \frac{e^{-\alpha y^2/(2\eta_\varepsilon)}}{\int_{-1}^{y} e^{-\alpha s^2/(2\eta_\varepsilon)}\, ds}.$$

We propose to do this in two steps: first for $y \in [-1+\varepsilon^\kappa, 1]$, then for $y \in (-1, -1+\varepsilon^\kappa]$, where $\kappa = \beta/2$.

(1) $y \in [-1+\varepsilon^\kappa, 1]$: Thanks to assumption 1.1, we have for all $s \in [-1, 1]$

$$V(b_\varepsilon s) = -\alpha b_\varepsilon^2 s^2/2 + \theta_\varepsilon(s) b_\varepsilon^3 s^3,$$

with

$$\sup_{s\in[-1,1]} |\theta_\varepsilon(s)| \le \frac{1}{6} \sup_{x\in[-b_\varepsilon, b_\varepsilon]} V^{(3)}(x) \le C,$$

where C is a constant independent of ε. As a consequence, since $b_\varepsilon = \varepsilon^\beta$ and $\eta_\varepsilon = \varepsilon^{1-2\beta}$,

$$e^{V(b_\varepsilon s)/\varepsilon} = e^{-\alpha s^2/(2\eta_\varepsilon)} e^{\theta_\varepsilon(s) s^3 \varepsilon^{3\beta-1}}.$$

Now, we can write

$$e^{\theta_\varepsilon(s) s^3 \varepsilon^{3\beta-1}} = 1 + \delta_\varepsilon(s)\theta_\varepsilon(s) s^3 \varepsilon^{3\beta-1},$$

with

$$\sup_{s\in[-1,1]} |\delta_\varepsilon(s)| \le e^{C\varepsilon^{3\beta-1}} \le \tilde{C},$$

where $\tilde{C}$ is a constant independent of ε. For the sake of simplicity, we denote $\theta_\varepsilon(s)$ for $\delta_\varepsilon(s)\theta_\varepsilon(s)$. This leads to the following decomposition

$$\frac{h_\varepsilon'(y)}{h_\varepsilon(y)} = \frac{1}{1 + \frac{\int_{-1}^{y} e^{-\alpha s^2/(2\eta_\varepsilon)} \theta_\varepsilon(s) s^3 \varepsilon^{3\beta-1}\, ds}{\int_{-1}^{y} e^{-\alpha s^2/(2\eta_\varepsilon)}\, ds}} \times \frac{e^{-\alpha y^2/(2\eta_\varepsilon)}}{\int_{-1}^{y} e^{-\alpha s^2/(2\eta_\varepsilon)}\, ds} \left(1 + \theta_\varepsilon(y) y^3 \varepsilon^{3\beta-1}\right).$$

Now, let us notice that for any $y \in (-1, 1]$,

$$\left| \frac{\int_{-1}^{y} e^{-\alpha s^2/(2\eta_\varepsilon)} \theta_\varepsilon(s) s^3 \varepsilon^{3\beta-1}\, ds}{\int_{-1}^{y} e^{-\alpha s^2/(2\eta_\varepsilon)}\, ds} \right| \le D\varepsilon^{3\beta-1},$$

with D independent of ε. Consequently,

$$\frac{1}{1 + \frac{\int_{-1}^{y} e^{-\alpha s^2/(2\eta_\varepsilon)} \theta_\varepsilon(s) s^3 \varepsilon^{3\beta-1}\, ds}{\int_{-1}^{y} e^{-\alpha s^2/(2\eta_\varepsilon)}\, ds}} = 1 - \lambda_\varepsilon(y)\varepsilon^{3\beta-1},$$

and there exists a constant E, independent of ε, such that

$$\sup_{y\in(-1,1]} |\lambda_\varepsilon(y)| < E.$$

Thus we can write

$$\frac{h_\varepsilon'(y)}{h_\varepsilon(y)} = \left(1 + \nu_\varepsilon(y)\varepsilon^{3\beta-1}\right) \times \frac{e^{-\alpha y^2/(2\eta_\varepsilon)}}{\int_{-1}^{y} e^{-\alpha s^2/(2\eta_\varepsilon)}\, ds},$$

and there exists a constant F, independent of ε, such that

$$\sup_{y\in(-1,1]} |\nu_\varepsilon(y)| < F.$$

Finally, for all $y \in (-1,1]$, we have obtained

$$|\Delta_\varepsilon(y)| := \left|\frac{h_\varepsilon'(y)}{h_\varepsilon(y)} - \frac{g_\varepsilon'(y)}{g_\varepsilon(y)}\right| \leq F\varepsilon^{3\beta-1} \times \frac{e^{-\alpha y^2/(2\eta_\varepsilon)}}{\int_{-1}^{y} e^{-\alpha s^2/(2\eta_\varepsilon)}\,ds}, \tag{4.4}$$

and the goal is now to upper-bound the last term in this equation. In this aim, we first consider the case where $y \in [-1+\varepsilon^\kappa, 0]$. In the integral, we make the change of variable

$$v = \varepsilon^{-\gamma} \times \frac{s^2 - y^2}{2\eta_\varepsilon},$$

with $\gamma = (5\beta-2)/2$, so that $\gamma > 0$ as soon as $\beta > 2/5$. We get

$$\int_{-1}^{y} e^{-\alpha s^2/(2\eta_\varepsilon)}\,ds = \eta_\varepsilon \varepsilon^\gamma e^{-\alpha y^2/(2\eta_\varepsilon)} I_\varepsilon(y),$$

where

$$I_\varepsilon(y) := \int_0^{\frac{\varepsilon^{-\gamma}(1-y^2)}{(2\eta_\varepsilon)}} \frac{e^{-\alpha\varepsilon^\gamma v}}{\sqrt{2\eta_\varepsilon\varepsilon^\gamma v + y^2}}\,dv.$$

Since $\eta_\varepsilon \varepsilon^\gamma = \varepsilon^{\beta/2}$ and $y \in [-1+\varepsilon^\kappa, 0]$, with $\kappa = \beta/2$, it is clear that for ε small enough, one has: $\forall y \in [-1+\varepsilon^\kappa, 1]$,

$$I_\varepsilon(y) \geq J_\varepsilon := \int_0^{1/2} \frac{e^{-\alpha\varepsilon^\gamma v}}{\sqrt{2\varepsilon^{\beta/2} v + 1}}\,dv \xrightarrow[\varepsilon\to 0]{} \frac{1}{2},$$

so that for ε small enough, one has $I_\varepsilon(y) \geq 1/4$. Putting all things together gives

$$|\Delta_\varepsilon(y)| \leq 4F\varepsilon^{3\beta-1} \times \varepsilon^{-\beta/2} = 4F\varepsilon^\gamma \xrightarrow[\varepsilon\to 0]{} 0,$$

and the uniform convergence is proved for $y \in [-1+\varepsilon^\kappa, 0]$. In order to conclude for $y \in [-1+\varepsilon^\kappa, 1]$, it remains to notice that if $y \in [0,1]$, one has

$$\frac{e^{-\alpha y^2/(2\eta_\varepsilon)}}{\int_{-1}^{y} e^{-\alpha s^2/(2\eta_\varepsilon)}\,ds} \leq \frac{1}{\int_{-1}^{0} e^{-\alpha s^2/(2\eta_\varepsilon)}\,ds} \underset{\varepsilon\to 0}{\sim} \sqrt{\frac{2\alpha}{\pi\eta_\varepsilon}}.$$

Coming back to Equation (4.4) yields, for all $y \in [0,1]$ and for ε small enough,

$$|\Delta_\varepsilon(y)| \leq F\varepsilon^{3\beta-1} \times \varepsilon^{\beta-1/2} = F\varepsilon^{4\beta-3/2} \xrightarrow[\varepsilon\to 0]{} 0,$$

since $\beta > 2/5$. This concludes the case where $y \in [-1+\varepsilon^\kappa, 1]$.

(2) $y \in (-1, -1+\varepsilon^\kappa]$: let us denote $y = -1 + p\varepsilon^\kappa$, with $0 < p \leq 1$, so that our goal is now to upper-bound

$$|\Delta_\varepsilon(p)| := \left|\frac{h_\varepsilon'(-1+p\varepsilon^\kappa)}{h_\varepsilon(-1+p\varepsilon^\kappa)} - \frac{g_\varepsilon'(-1+p\varepsilon^\kappa)}{g_\varepsilon(-1+p\varepsilon^\kappa)}\right|,$$

that is to say

$$|\Delta_\varepsilon(p)| = \left|\frac{e^{V(b_\varepsilon(-1+p\varepsilon^\kappa))/\varepsilon}}{\int_{-1}^{-1+p\varepsilon^\kappa} e^{V(b_\varepsilon s)/\varepsilon}\,ds} - \frac{e^{-\alpha(-1+p\varepsilon^\kappa)^2/(2\eta_\varepsilon)}}{\int_{-1}^{-1+p\varepsilon^\kappa} e^{-\alpha s^2/(2\eta_\varepsilon)}\,ds}\right|,$$

independently of $p \in (0,1]$. For any smooth function f on $[-1,0]$, we may write the following Taylor expansions

$$f(-1+p\varepsilon^\kappa) = f(-1) + f'(-1)p\varepsilon^\kappa + \frac{f''(\theta_1)}{2}p^2\varepsilon^{2\kappa},$$

and

$$\int_{-1}^{-1+p\varepsilon^{\kappa}} f(s)\,ds = f(-1)p\varepsilon^{\kappa} + \frac{f'(-1)}{2}p^2\varepsilon^{2\kappa} + \frac{f''(\theta_2)}{6}p^3\varepsilon^{3\kappa},$$

where θ_1 and θ_2 belong to the interval $(-1,-1+\varepsilon^{\kappa})$, and depend on p and ε. This leads to

$$\frac{f(-1+p\varepsilon^{\kappa})}{\int_{-1}^{-1+p\varepsilon^{\kappa}} f(s)\,ds} = \frac{1}{p\varepsilon^{\kappa}} \times \frac{1+\frac{f'(-1)}{f(-1)}p\varepsilon^{\kappa} + \frac{1}{2}\frac{f''(\theta_1)}{f(-1)}p^2\varepsilon^{2\kappa}}{1+\frac{1}{2}\frac{f'(-1)}{f(-1)}p\varepsilon^{\kappa} + \frac{1}{6}\frac{f''(\theta_2)}{f(-1)}p^2\varepsilon^{2\kappa}}.$$

Considering $f(s) = e^{-\alpha s^2/(2\eta_\varepsilon)}$, we get

$$\frac{f'(-1)}{f(-1)}p\varepsilon^{\kappa} = \alpha p\varepsilon^{\beta/2}\varepsilon^{-1+2\beta} = \alpha p\varepsilon^{\gamma},$$

and

$$\frac{f''(\theta)}{f(-1)}p^2\varepsilon^{2\kappa} = p^2\left(\frac{\alpha^2\theta^2}{\eta_\varepsilon^2} - \frac{\alpha}{\eta_\varepsilon}\right)\varepsilon^{2\kappa}e^{\alpha(1-\theta^2)/(2\eta_\varepsilon)}.$$

Now, since $\theta \in (-1,-1+\varepsilon^{\kappa})$, then $0 \le 1-\theta^2 \le 2\varepsilon^{\kappa}$ and, uniformly w.r.t θ,

$$e^{\alpha(1-\theta^2)/(2\eta_\varepsilon)} \xrightarrow[\varepsilon\to 0]{} 1 \quad \text{and} \quad \frac{f''(\theta)}{f(-1)}p^2\varepsilon^{2\kappa} \underset{\varepsilon\to 0}{\sim} \alpha^2p^2\varepsilon^{2\gamma}.$$

Thus we have the following Taylor expansion

$$\frac{f(-1+p\varepsilon^{\kappa})}{\int_{-1}^{-1+p\varepsilon^{\kappa}} f(s)\,ds} = \frac{1}{p\varepsilon^{\kappa}} \times \left(1+\frac{\alpha p}{2}\varepsilon^{\gamma} + \phi_\varepsilon(p)p\varepsilon^{2\gamma}\right),$$

with $\sup_{0<p\le 1}|\phi_\varepsilon(p)| < \infty$. Considering this time $f(s) = e^{V(b_\varepsilon s)/\varepsilon}$, we get

$$\frac{f'(-1)}{f(-1)}p\varepsilon^{\kappa} = p\varepsilon^{\kappa} \times \frac{b_\varepsilon V'(-b_\varepsilon)}{\varepsilon} = \alpha p\varepsilon^{\gamma} + \xi_\varepsilon(p)\varepsilon^{\gamma+\beta},$$

and

$$\frac{f''(\theta)}{f(-1)}p^2\varepsilon^{2\kappa} = p^2\left(\left(\frac{b_\varepsilon V'(b_\varepsilon\theta)}{\varepsilon}\right)^2 + \frac{b_\varepsilon^2 V''(b_\varepsilon\theta)}{\varepsilon}\right)\varepsilon^{2\kappa}e^{(V(b_\varepsilon\theta)-V(-b_\varepsilon))/\varepsilon}.$$

For the same reason as above, we have then

$$\frac{f''(\theta)}{f(-1)}p^2\varepsilon^{2\kappa} \underset{\varepsilon\to 0}{\sim} \alpha^2p^2\varepsilon^{2\gamma}.$$

Since $\beta > \gamma$, we have the following Taylor expansion

$$\frac{f(-1+p\varepsilon^{\kappa})}{\int_{-1}^{-1+p\varepsilon^{\kappa}} f(s)\,ds} = \frac{1}{p\varepsilon^{\kappa}} \times \left(1+\frac{\alpha p}{2}\varepsilon^{\gamma} + \varphi_\varepsilon(p)p\varepsilon^{2\gamma}\right),$$

with $\sup_{0<p\le 1}|\varphi_\varepsilon(p)| < \infty$. Gathering the intermediate results, we get

$$|\Delta_\varepsilon(p)| = |\varphi_\varepsilon(p) - \phi_\varepsilon(p)|\varepsilon^{2\gamma-\kappa} \le G\varepsilon^{(9\beta-4)/2},$$

where G is independent of ε. It turns out that the uniform convergence is ensured as soon as $\beta > 4/9$.

This concludes the proof of Lemma 4.9.

□

Step 6. The difference of the two drifts in (4.3) is negligible with respect to the variance η_ε of the Brownian component as soon as $4/9 < \beta < 1/2$. Theorem 4.3 in Day (1992) ensures that $\mathcal{L}(Y_\cdot|T_1 < T_{-1})$ and $\mathcal{L}(Z_\cdot|T_1 < T_{-1})$ are then asymptotically equivalent. This approximation result relies on the Girsanov Theorem. The Novikov condition ensuring that the exponential martingale is uniformly integrable can be checked as in Day (1992). In particular, a consequence of the results in Day (1992) is that, in the limit $\varepsilon \to 0$, T_1^Y and T_1^Z have the same law.
Step 7. After an obvious scaling, we have to estimate the reactive time for a repulsive Ornstein-Uhlenbeck process between $-b_\varepsilon$ and b_ε starting at

$$x_\varepsilon = -c_\varepsilon = -\varepsilon^\gamma \xrightarrow[\varepsilon\to 0]{} 0.$$

Since $b_\varepsilon/\sqrt{\varepsilon}$ and $c_\varepsilon/\sqrt{\varepsilon}$ both go to infinity when ε goes to zero, the estimates in the proof of Theorem 3.3 (see also Remark 3.5) ensure that

$$T_1^Z + \frac{1}{\alpha}(\log\varepsilon - \log c_\varepsilon - \log b_\varepsilon) \xrightarrow[\varepsilon\to 0]{\mathcal{L}} \frac{1}{\alpha}(G - \log\alpha),$$

where the law of G is a standard Gumbel distribution. Putting all things together, we have established the following estimate.

Proposition 4.10. *Conditionally to the event* $\{T_{b_\varepsilon} < T_A\}$,

$$T_{-c_\varepsilon\to b_\varepsilon} + \frac{1}{\alpha}(\log\varepsilon - \log c_\varepsilon - \log b_\varepsilon) \xrightarrow[\varepsilon\to 0]{\mathcal{L}} \frac{1}{\alpha}(G - \log\alpha),$$

where the law of G is a standard Gumbel distribution.

4.4. *Conclusion.* The estimates of Propositions 4.1 and 4.10 are the key points of the proof of Theorem 1.4.

Proof of Theorem 1.4: One can write

$$-\int_{b_\varepsilon}^B \frac{ds}{V'(s)} = -\frac{1}{\alpha}\left(\int_{b_\varepsilon}^B \left(\frac{\alpha}{V'(s)} + \frac{1}{s}\right) ds - \int_{b_\varepsilon}^B \frac{ds}{s}\right)$$

Thanks to Assumption 1.1, $s \mapsto \alpha V'(s)^{-1} + s^{-1}$ is integrable on $(0, B)$.

$$t_{b_\varepsilon\to B} = -\frac{\log b_\varepsilon}{\alpha} + \frac{\log B}{\alpha} - \frac{1}{\alpha}\int_0^B \left(\frac{\alpha}{V'(s)} + \frac{1}{s}\right) ds + o_\varepsilon(1).$$

Similarly,

$$t_{-c_\varepsilon\to x} = -\frac{\log c_\varepsilon}{\alpha} + \frac{\log|x|}{\alpha} + \frac{1}{\alpha}\int_x^0 \left(\frac{\alpha}{V'(s)} + \frac{1}{s}\right) ds + o_\varepsilon(1).$$

Using the fact that

$$T_{x\to B} = T_{x\to -c_\varepsilon} + T_{-c_\varepsilon\to b_\varepsilon} + T_{b_\varepsilon\to B},$$

Propositions 4.1 and 4.10 and the two previous estimates on $t_{b_\varepsilon\to B}$ and $t_{-c_\varepsilon\to x}$ imply that for any $x \in (A, 0)$, conditionally to $\{T_B < T_A\}$,

$$T_{x\to B} + \frac{1}{\alpha}\log\varepsilon \xrightarrow[\varepsilon\to 0]{\mathcal{L}} \frac{1}{\alpha}(\log(|x|B) + F(x) + F(B) - \log\alpha + G).$$

This concludes the proof of Theorem 1.4. Notice that one can let x go to A in this expression. $\square$

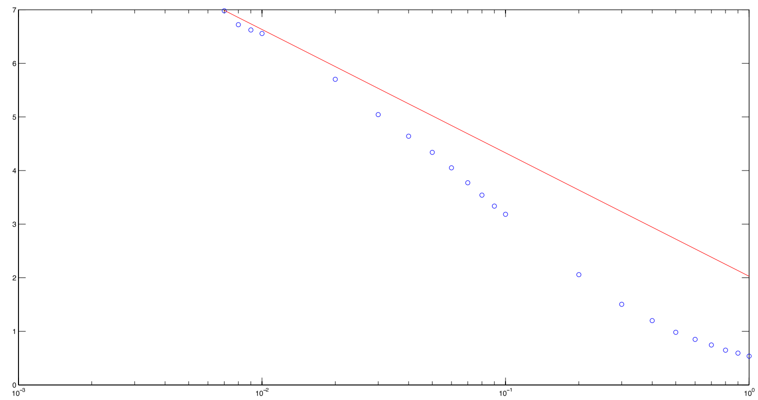

Figure 4.4. Mean time of the reactive path for the potential V given in (1.6) as a function of $\log\varepsilon$. The 95% confidence intervals are of the size of the points. These results have been obtained with the algorithm described in Cérou et al. (2011). The theoretical asymptotic behavior (when ε goes to 0) is drawn in red.

Figure 4.4 illustrates this result for the process

$$dX_t^{(\varepsilon)} = -V'(X_t^{(\varepsilon)})\,dt + \sqrt{2\varepsilon}dB_t,$$

with $V(x) = x^4/4 - x^2/2$, $X_0^{(\varepsilon)} = x = -0.89$, on the set $[A, B] = [-0.9, 0.9]$. Denoting $T_{-0.89\to 0.9}$ the length of the reactive path from -0.89 to 0.9, then Theorem 1.4 ensures that, when ε goes to zero, $\mathbb{E}[T_{-0.89\to 0.9}]$ is equivalent to

$$-\log\varepsilon + \log(0.89\times 0.9) - \frac{1}{2}\log(1-0.89^2) - \frac{1}{2}\log(1-0.9^2) + \gamma,$$

where γ stands for Euler's constant. Figure 4.4 compares this theoretical result (continuous line) with the empirical means obtained thanks to the algorithm described in Cérou et al. (2011) for ε ranging from 0.007 to 1 (circles).

5. Other examples

The aim of this section is to analyze the distribution of the lengths of the reactive paths, when the potential V has a maximum at point $z^* = 0$, but does not satisfy Assumption 1.1. More precisely, we successively consider three cases:

(1) V behaves like $-|x|$ around $x = 0$,
(2) V is constant equal to 0 around $x = 0$,
(3) V is regular at 0 but $V''(0) = 0$.

We will derive explicit expressions for the distributions of the lengths of the reactive paths in the asymptotic regime ε goes to 0. In all these cases, it turns out that the asymptotic behaviors are very different from what we obtained in Theorem 1.4.

5.1. *Brownian motion with drift.* The easiest case to deal with is the one of the singular potential $V(x) = -\beta|x|$. It corresponds to a Brownian motion with a piecewise constant drift, namely:

$$dX_t^{(\varepsilon)} = \beta \operatorname{sgn}\left(X_t^{(\varepsilon)}\right)\,dt + \sqrt{2\varepsilon}dB_t,$$

where β is a positive real number and $\mathrm{sgn}(x)$ stands for the sign of x (see for example Veretennikov (1980); Gyöngy and Krylov (1996) for the existence and uniqueness of strong solutions to this stochastic differential equation). In that case, Equation (2.2) is a second order ordinary differential equation with constant coefficients.

Let us recall the expression of the Laplace transform of the conditioned first exit time on (a, b) for a Brownian motion with drift (see Borodin and Salminen (2002, p.309)).

Proposition 5.1. *Choose $a < x < b$, $\mu \in \mathbb{R}$, and consider the process $W^{(\mu)}$ defined by $W_t^{(\mu)} = \mu t + W_t$. Let us denote by H the first exit time of (a, b). Then,*

$$\mathbb{E}_x\left(e^{-sH} | W_H^{(\mu)} = b\right) = \frac{\sinh((b-a)|\mu|)}{\sinh((x-a)|\mu|)} \frac{\sinh((x-a)\sqrt{2s+\mu^2})}{\sinh((b-a)\sqrt{2s+\mu^2})}.$$

A few remarks are in order.

Remark 5.2. Notice that the law of H knowing that $T_b < T_a$ does not depend on the sign of the drift μ. This may seem surprising at first sight but it is consistent with the fact that going up is equivalent to going down after introducing the h-transformed process, see Section 4.2 above.

Remark 5.3. Notice that

$$\lim_{x \to a} \mathbb{E}_x\left(e^{-sH} | W_H^{(\mu)} = b\right) = \frac{\sinh((b-a)|\mu|)}{|\mu|} \frac{\sqrt{2s+\mu^2}}{\sinh((b-a)\sqrt{2s+\mu^2})}. \tag{5.1}$$

Remark 5.4. If $\mu > 0$, then H converges to H_b the hitting time of b as $a \to -\infty$:

$$\lim_{a \to -\infty} \mathbb{E}_x\left(e^{-sH} | W_H^{(\mu)} = b\right) = e^{\mu(b-x)(1-\sqrt{1+2s/\mu^2})},$$

which is the Laplace transform of the inverse Gaussian distribution with parameter $m = (b-x)/\mu$ and $\ell = m^2$. We recall that the density of the inverse Gaussian distribution with parameters (m, ℓ) is

$$f(x) = \sqrt{\frac{\ell}{2\pi}}\, x^{-3/2} \exp\left(-\frac{\ell(x-m)^2}{2m^2 x}\right) \mathbb{1}_{\{x>0\}}.$$

We can use these results to study the law of the hitting of 0 starting from $x = -\delta$ if the process $X^{(\varepsilon)}$ satisfies, at least when $X_t^{(\varepsilon)} \in (-\delta, 0)$:

$$X_t^{(\varepsilon)} = x + \sqrt{2\varepsilon} B_t - \beta t.$$

From the scaling property of the Brownian motion, we can compute the Laplace transform F of $H = \inf\left\{t \geq 0 \ : \ X_t^{(\varepsilon)} \notin (-\delta, 0)\right\}$ conditionally to $\left\{X_H^{(\varepsilon)} = 0\right\}$, using (5.1):

$$\begin{aligned} F_\varepsilon(s) &= \frac{\sinh(\delta\beta/(2\varepsilon))}{\sinh(\delta\sqrt{\beta^2/(2\varepsilon)^2 + s/\varepsilon})} \frac{\sqrt{\beta^2/(2\varepsilon)^2 + s/\varepsilon}}{\beta/(2\varepsilon)} \\ &= \frac{\exp\left(\frac{\delta\beta}{2\varepsilon}\left(1 - \sqrt{1 + \frac{4\varepsilon s}{\beta^2}}\right)\right) - \exp\left(-\frac{\delta\beta}{2\varepsilon}\left(1 + \sqrt{1 + \frac{4\varepsilon s}{\beta^2}}\right)\right)}{1 - \exp\left(-\frac{\delta\beta}{\varepsilon}\sqrt{1 + \frac{4\varepsilon s}{\beta^2}}\right)} \sqrt{1 + \frac{4\varepsilon s}{\beta^2}}. \end{aligned}$$

For a fixed s, we thus get $\lim_{\varepsilon\to 0} F_\varepsilon(s) = \exp\left(-\frac{\delta s}{\beta}\right)$, and

$$\begin{aligned}
\mathbb{E}\left(\exp\left(-s\frac{H-\delta/\beta}{\sqrt{\varepsilon}}\right)\right) &= \exp\left(\frac{s\delta/\beta}{\sqrt{\varepsilon}}\right) F_\varepsilon(s/\sqrt{\varepsilon}) \\
&= \frac{\exp\left(\frac{s\delta}{\beta\sqrt{\varepsilon}}\right)}{\sqrt{1+\frac{4\sqrt{\varepsilon}s}{\beta^2}}} \frac{\exp\left(\frac{\delta\beta}{2\varepsilon}\left(1-\sqrt{1+\frac{4\sqrt{\varepsilon}s}{\beta^2}}\right)\right) - \exp\left(-\frac{\delta\beta}{2\varepsilon}\left(1+\sqrt{1+\frac{4\sqrt{\varepsilon}s}{\beta^2}}\right)\right)}{1-\exp\left(-\frac{\delta\beta}{\varepsilon}\sqrt{1+\frac{4\sqrt{\varepsilon}s}{\beta^2}}\right)} \\
&\underset{\varepsilon\to 0}{\sim} \exp\left(\frac{s\delta}{\beta\sqrt{\varepsilon}} + \frac{\delta\beta}{2\varepsilon}\left(1-1-\frac{2\sqrt{\varepsilon}s}{\beta^2}+\frac{2\varepsilon s^2}{\beta^4}\right)\right) \\
&\underset{\varepsilon\to 0}{\sim} \exp\left(\frac{\delta s^2}{\beta^3}\right).
\end{aligned}$$

As a consequence,

$$H \xrightarrow[\varepsilon\to 0]{a.s.} \frac{\delta}{\beta} \quad \text{and} \quad \frac{H-\delta/\beta}{\sqrt{\varepsilon}} \xrightarrow[\varepsilon\to 0]{\mathcal{L}} \mathcal{N}\left(0, \frac{2\delta}{\beta^3}\right).$$

In this case, with the same reasoning as in Section 4.1, one can deduce that the length of the reactive path between points $-\delta$ and $+\delta$ has the deterministic limit $2\delta/\beta$ when ε tends to zero. The absence of any asymptotic randomness in the length of the reactive path, in contrast with Theorem 1.4, is due to the fact that in this case, we do not have $V'(0) = 0$. The next situation that we propose to deal with is the opposite one, specifically when $V'(x) = 0$ in a neighborhood of 0, and we call it the totally flat potential.

5.2. *Totally flat potential.* Let us investigate in this section the case when the potential V is flat around the saddle point. Specifically, let us consider the process given by $X_t^{(\varepsilon)} = \sqrt{2\varepsilon} B_t$, $b > 0$ and

$$H = \inf\left\{t > 0,\ X_t^{(\varepsilon)} \notin (-b, b)\right\}.$$

One has, for any $s \geq 0$,

$$F_\varepsilon(s) = \mathbb{E}_{-b}\left(e^{-sH} | X_H^{(\varepsilon)} = b\right) = \frac{\sqrt{4b^2 s/\varepsilon}}{\sinh\left(\sqrt{4b^2 s/\varepsilon}\right)}.$$

Moreover,

$$\mathbb{E}_{-b}\left(e^{sH} | X_H^{(\varepsilon)} = b\right) = \frac{\sqrt{4b^2 s/\varepsilon}}{\sin\left(\sqrt{4b^2 s/\varepsilon}\right)} \quad \text{if } 0 \leq s \leq \frac{\pi^2}{4b^2}\varepsilon.$$

Notice that, for any $s \in \left[0, \frac{\pi^2}{4b^2}\varepsilon\right]$,

$$\mathbb{E}_{-b}\left(e^{sH} | X_H^{(\varepsilon)} = b\right) = G\left(\frac{4b^2 s}{\varepsilon}\right) \quad \text{where} \quad G(x) = \frac{1}{\sum_{k\geq 0} \frac{(-x)^k}{(2k+1)!}}.$$

In particular,

$$\mathbb{E}\left(H | X_H^{(\varepsilon)} = b\right) = \frac{2b^2}{3\varepsilon} \quad \text{and} \quad \mathbb{V}\left(H | X_H^{(\varepsilon)} = b\right) = \frac{8b^4}{45\varepsilon^2}.$$

Lemma 5.5 (Borodin and Salminen (2002)). *For any $\varepsilon > 0$ and $b > 0$, one has, conditionally to $X_0^{(\varepsilon)} = x$ and $T_b < T_{-b}$, and in the limit $x \to -b$,*

$$H_{-b,b}^{(\varepsilon)} = \frac{b^2}{\varepsilon}\left(\frac{2}{3} + \frac{2\sqrt{2}}{3\sqrt{5}}Y\right),$$

where $\mathbb{E}(Y) = 0$, $\mathbb{V}(Y) = 1$, and its Laplace transform is given by

$$\mathbb{E}\big(e^{-sY}\big) = \frac{\sqrt{As}}{\sinh\left(\sqrt{As}\right)}e^{Bs} \quad \textit{where} \quad A = \frac{6\sqrt{5}}{\sqrt{2}} \quad \textit{and} \quad B = \frac{\sqrt{5}}{\sqrt{2}}.$$

In conclusion, in the case of a totally flat potential, the length of a reactive path goes to infinity at rate $1/\varepsilon$ when ε goes to zero. Again, this is different from the non-degenerate case of Theorem 1.4 where the length of a reactive path goes to infinity at a slower rate, namely $\log(1/\varepsilon)$ (if $V''(0) = -1$).

5.3. *Degenerate concave potentials.* Between the two extreme situations of Section 5.1 (where $V'(0) \neq 0$) and Section 5.2 (totally flat potential), the main result of this paper stated in Theorem 1.4 studies the length of a reactive path for a potential V which is non-degenerate at 0 (also called quadratic case: $V'(0) = 0$ but $V''(0) \neq 0$). In this last section, we briefly discuss some intermediate situations, when the second derivative of the potential V is equal to 0 at the local maximum 0. Again, we will see that the asymptotic of the length of the reactive path is very different from the quadratic case of Theorem 1.4. To that end, we focus on monomial potentials: the potential V is given by

$$V(x) = -\frac{x^{2n+2}}{2n+2} \quad \text{with} \quad n \geq 1.$$

We consider the diffusion process $(X_t^{(\varepsilon)})_{t\geq 0}$ solution of

$$X_t^{(\varepsilon)} = x + \sqrt{2\varepsilon}B_t + \int_0^t (X_s^{(\varepsilon)})^{2n+1}\,ds. \tag{5.2}$$

As will be explained below, in this case, the length of a reactive path goes to infinity at rate $\varepsilon^{-\frac{n}{n+1}}$ when ε goes to zero. Notice that when n goes to infinity, $\varepsilon^{-\frac{n}{n+1}}$ tends to $1/\varepsilon$, which is consistent with the scaling obtained in Section 5.2 for a totally flat potential.

For convenience, we drop in the sequel the parameter ε. Let us define

$$t_\varepsilon = \varepsilon^{-\frac{n}{n+1}}, \quad a_\varepsilon = \varepsilon^{\frac{1}{2n+2}}, \quad b_\varepsilon = \frac{b}{a_\varepsilon}, \quad x_\varepsilon = \frac{x}{a_\varepsilon},$$

and introduce the process $(\tilde{X}_t)_{t\geq 0}$ defined by

$$\tilde{X}_t = \frac{X_{t_\varepsilon t}}{a_\varepsilon}.$$

The process $(\tilde{X}_t)_{t\geq 0}$ is solution of the stochastic differential equation

$$\tilde{X}_t = x_\varepsilon + \sqrt{2}B_t + \int_0^t \tilde{X}_s^{2n+1}\,ds, \tag{5.3}$$

and we have that

$$\{T_b < T_{-b}\} = \left\{\tilde{T}_{b_\varepsilon} < \tilde{T}_{-b_\varepsilon}\right\},$$

with obvious notation. On this event, $T_b = t_\varepsilon \tilde{T}_{b_\varepsilon}$. In Equation (5.3), the parameter ε only appears in the boundary conditions as in Equation (3.4) for the Ornstein-Uhlenbeck process. Notice that, in the Ornstein-Uhlenbeck case ($n = 0$), t_ε is equal to 1. As in the Ornstein-Uhlenbeck case, conditionally to the event $\left\{\tilde{T}_{b_\varepsilon} < \tilde{T}_{-b_\varepsilon}\right\}$, $(\tilde{X}_t)_{t\geq 0}$ is still a Markov process starting from x_ε and solution of

$$dY_t = \sqrt{2}\,dB_t + f_\varepsilon(Y_t)\mathbb{1}_{\{\tilde{T}_{b_\varepsilon} > t\}}\,dt \quad \text{with} \quad f_\varepsilon(y) = -V'(y) + 2\frac{e^{V(y)}}{\int_{-b_\varepsilon}^{y} e^{V(s)}\,ds}.$$

Our goal is to show that, conditionally to $\left\{\tilde{T}_{b_\varepsilon} < \tilde{T}_{-b_\varepsilon}\right\}$, $\tilde{T}_{b_\varepsilon}$ has a limit in law when ε goes to zero. This will show that T_b (conditionally to the event $\{T_b < T_{-b}\}$) scales like $\varepsilon^{-\frac{n}{n+1}}$, which is the scaling announced above.

The idea is to compare $(Y_t)_{t\geq 0}$ to the solution $(Z_t)_{t\geq 0}$ of the following equation

$$dZ_t = \sqrt{2}dB_t + f(Z_t)\,dt \quad \text{with} \quad f(z) = -V'(z) + 2\frac{e^{V(z)}}{\int_{-\infty}^{z} e^{V(s)}\,ds}. \tag{5.4}$$

The following lemma ensures that $(Z_t)_{t\geq 0}$ goes to $+\infty$ in a finite (and integrable) time, even if it 'starts from $-\infty$'.

Lemma 5.6. *If $(Z_t)_{t\geq 0}$ is solution of Equation (5.4) starting from $x \in \mathbb{R}$, then it goes to $+\infty$ at a (random) finite time τ_e. Moreover, τ_e is integrable and it converges almost surely to an integrable random time when x goes to $-\infty$:*

$$\lim_{x\to-\infty} \mathbb{E}_x(\tau_e) = \int_{-\infty}^{+\infty} (p(+\infty) - p(y))m(y)\,dy < +\infty,$$

where

$$m(x) = \exp\left(\int_0^x f(z)\,dz\right) \quad \text{and} \quad p(x) = \int_0^x \exp\left(-\int_0^y f(z)\,dz\right)dy = \int_0^x \frac{dy}{m(y)}.$$

Proof of Lemma 5.6: The result on the longtime behavior of $(Z_t)_{t\geq 0}$ is a consequence of the behavior at infinity of the drift f given by Equation (5.4). For any $x < 0$, three successive integrations by parts lead to

$$0 \leq \int_{-\infty}^{x} e^{V(s)}\,ds + \frac{e^{V(x)}}{x^{2n+1}}\left(1 - \frac{2n+1}{x^{2n+2}}\right) \leq -(2n+1)(4n+3)\frac{e^{V(x)}}{x^{6n+5}}. \tag{5.5}$$

As a by-product, we get that for any $x < -(2n+1)^{\frac{1}{2n+2}}$,

$$0 < -x^{2n+1} \leq f(x) \leq -x^{2n+1}\left(\frac{2}{1 - \frac{2n+1}{x^{2n+2}}} - 1\right). \tag{5.6}$$

Let us introduce, for any $n \geq 1$,

$$C_n = \int_{-\infty}^{+\infty} e^{V(s)}\,ds = \int_{-\infty}^{+\infty} e^{\frac{-s^{2n+2}}{2n+2}}\,ds.$$

For any $x > 0$, we have

$$\int_{-\infty}^{x} e^{V(s)}\,ds = C_n - \int_{-\infty}^{-x} e^{V(s)}\,ds,$$

so that the previous computations imply that for any $x > 0$ sufficiently large so that $\frac{e^{V(x)}}{x^{2n+1}} < C_n$, we have

$$0 < x^{2n+1} \leq f(x) \leq x^{2n+1} + \frac{2e^{V(x)}}{C_n - \frac{e^{V(x)}}{x^{2n+1}}}. \tag{5.7}$$

A quick inspection of the estimates (5.6) and (5.7) indicates in particular that

$$f(x) \underset{|x|\to+\infty}{\sim} |x|^{2n+1}.$$

As a consequence, the process $(Z_t)_{t\geq 0}$ starting from $x \in \mathbb{R}$ explodes with probability 1 at a (random) finite time τ_e and $Z_t \to +\infty$ as $t \to \tau_e$ (see for instance Karatzas and Shreve (1991, ch.6)). In short, this is a straightforward consequence of the expression of $\mathbb{E}_x(T_a \wedge T_b)$ that can be found in Karatzas and Shreve (1991, ch.6) and the fact that $1/f(x)$ is integrable at $\pm\infty$. Indeed, for any $x \in (a, b)$,

$$\mathbb{E}_x(T_a \wedge T_b) = -\int_a^x (p(x) - p(y))m(y)\,dy + \frac{p(x) - p(a)}{p(b) - p(a)} \int_a^b (p(b) - p(y))m(y)\,dy,$$

with

$$m(x) = \exp\left(\int_0^x f(z)\,dz\right) \quad \text{and} \quad p(x) = \int_0^x \frac{dy}{m(y)}.$$

One has obviously that $p(b) \to p(+\infty) \in (0, +\infty)$ as $b \to +\infty$, and $p(a) \to -\infty$ as $a \to -\infty$. Thus,

$$\lim_{\substack{a\to-\infty \\ b\to+\infty}} \frac{p(x) - p(a)}{p(b) - p(a)} \int_a^b (p(b) - p(y))m(y)\,dy = \int_\infty^\infty (p(+\infty) - p(y))m(y)\,dy \in (0, +\infty].$$

Now, to show that τ_e is integrable (including in the limit $x \to -\infty$), we need to prove that

$$\int_{-\infty}^{+\infty} (p(+\infty) - p(y))m(y)\,dy < +\infty.$$

In this aim, let us first notice that for any real number y, we have

$$\begin{aligned}(p(+\infty) - p(y))m(y) &= \left(\int_y^{+\infty} \exp\left(-\int_0^x f(s)\,ds\right)dx\right) \times \exp\left(\int_0^y f(s)\,ds\right) \\ &= \int_y^{+\infty} \exp\left(-\int_y^x f(s)\,ds\right)dx.\end{aligned}$$

From the definition of f, one clearly has $f(s) \geq s^{2n+1}$ for any $s \in \mathbb{R}$. Hence, for any $y > 0$,

$$0 \leq (p(+\infty) - p(y))m(y) \leq e^{\frac{y^{2n+2}}{2n+2}} \int_y^{+\infty} e^{\frac{-x^{2n+2}}{2n+2}}\,dx.$$

The symmetry of the potential V and an integration by parts show that for any $y > 0$,

$$\int_y^{+\infty} e^{\frac{-x^{2n+2}}{2n+2}}\,dx = \int_{-\infty}^{-y} e^{V(s)}\,ds \leq \frac{e^{\frac{-y^{2n+2}}{2n+2}}}{y^{2n+1}},$$

so that

$$0 \leq (p(+\infty) - p(y))m(y) \leq \frac{1}{y^{2n+1}}.$$

Since $n \geq 1$, the integrability of the function $y \mapsto (p(+\infty) - p(y))m(y)$ when y tends to $+\infty$ is established. In order to conclude, we have to estimate this quantity when y goes to $-\infty$ as well. For this, let us first recall that

$$f(s) \underset{s\to-\infty}{\sim} |s|^{2n+1},$$

so that $p(+\infty)m(y)$ is clearly integrable when y goes to $-\infty$. The estimation of the remaining term is slightly more involved. We rewrite it as follows

$$-p(y)m(y) = -m(y)\int_0^y \exp(-F(x))\,dx,$$

where for any real number x, we define $F(x)$ as the primitive of f with value 0 at 0

$$F(x) = \int_0^x f(s)\,ds.$$

Notice that $\lim_{x\to-\infty} F(x) = -\infty$. Then an integration by parts gives

$$\int_0^y \exp(-F(x))\,dx = \frac{C_n}{4} - \frac{\exp(-F(y)}{f(y)} - \int_0^y \frac{f'(x)}{f(x)^2}\exp(-F(x))\,dx. \tag{5.8}$$

Next, we focus on the last term of this equation, namely

$$\int_0^y \frac{f'(x)}{f(x)^2}\exp(-F(x))\,dx.$$

For this, we first deduce from the definition of f that

$$f'(x) = -V''(x) + 2\frac{e^{V(x)}}{\int_{-\infty}^x e^{V(s)}\,ds}\left(V'(x) - \frac{e^{V(x)}}{\int_{-\infty}^x e^{V(s)}\,ds}\right).$$

From Equation (5.5), we know that

$$\frac{e^{V(x)}}{\int_{-\infty}^x e^{V(s)}\,ds} \underset{x\to-\infty}{\sim} |x|^{2n+1},$$

and more precisely that

$$V'(x) - \frac{e^{V(x)}}{\int_{-\infty}^x e^{V(s)}\,ds} \underset{x\to-\infty}{\sim} \frac{-(2n+1)}{|x|}.$$

This leads to

$$f'(x) \underset{x\to-\infty}{\sim} -(2n+1)x^{2n},$$

and

$$\frac{f'(x)}{f(x)^2}\exp(-F(x)) \underset{x\to-\infty}{\sim} \frac{-(2n+1)}{x^{2n+2}}\exp(-F(x)).$$

From this we deduce

$$\int_{-\infty}^0 \frac{f'(x)}{f(x)^2}\exp(-F(x))\,dx = -\infty.$$

Since $\frac{f'(x)}{f(x)^2}\exp(-F(x)) = o(\exp(-F(x)))$ when x tends to $-\infty$, we have

$$\int_0^y \frac{f'(x)}{f(x)^2}\exp(-F(x))\,dx \underset{y\to-\infty}{=} o\left(\int_0^y \exp(-F(x))\,dx\right),$$

and coming back to Equation (5.8) gives the following asymptotics

$$\int_0^y \exp(-F(x))\,dx \underset{y\to-\infty}{\sim} \frac{-\exp(-F(y))}{f(y)},$$

so that

$$-m(y)\int_0^y \exp(-F(x))\,dx \underset{y\to-\infty}{\sim} \frac{1}{f(y)} \underset{y\to-\infty}{\sim} \frac{1}{|y|^{2n+1}}.$$

To sum up, we have shown that

$$\int_{-\infty}^{+\infty}(p(+\infty)-p(y))m(y)\,dy < +\infty.$$

This ensures that

$$\begin{aligned}\mathbb{E}_x(\tau_e) &= \lim_{\substack{a\to-\infty\\ b\to+\infty}} \mathbb{E}_x(T_a\wedge T_b)\\ &= -\int_{-\infty}^{x}(p(x)-p(y))m(y)\,dy + \int_{-\infty}^{+\infty}(p(+\infty)-p(y))m(y)\,dy.\end{aligned}$$

In particular, $\mathbb{E}_x(\tau_e)$ is finite for any $x\in\mathbb{R}$. Finally, by the monotone convergence theorem, τ_e has a limit almost surely when $x\to-\infty$ and

$$\lim_{x\to-\infty}\mathbb{E}_x(\tau_e) = \int_{-\infty}^{+\infty}(p(+\infty)-p(y))m(y)\,dy < +\infty.$$

This concludes the proof of Lemma 5.6. □

Thanks to Lemma 5.6, we see that $T^Z_{a\to b}$ converges almost surely to a positive and integrable random variable T^Z_∞ as $a\to-\infty$ and $b\to+\infty$. Moreover,

$$\mathbb{E}(T^Z_\infty) = \int_{-\infty}^{+\infty}(p(+\infty)-p(y))m(y)\,dy < +\infty.$$

Now, notice that the drift f_ε that drives Y is greater than f. This ensures that if $Z_0 = Y_0$ then, almost surely, $Z_t \le Y_t$, for any $t\in[0,\tilde{T}_{b_\varepsilon})$. As a consequence, for any $x\in(-b_\varepsilon, b)$, one has $T^Y_{x\to b} \le T^Z_{x\to b}$. By monotone convergence, $T^Y_{x_\varepsilon\to b_\varepsilon}$ converges to a random variable which is integrable since

$$\mathbb{E}\big(T^Y_{x_\varepsilon\to b_\varepsilon}\big) \le \mathbb{E}\big(T^Z_\infty\big) < \infty.$$

To prove this result with full details, one would need to cut reactive trajectories into pieces, as done in Section 4 above for the quadratic case. This concludes the proof of the fact that $\tilde{T}_{b_\varepsilon}$, conditionally to $\left\{\tilde{T}_{b_\varepsilon} < \tilde{T}_{-b_\varepsilon}\right\}$, has a limit in law when ε goes to zero, and consequently, that T_b (conditionally to the event $\{T_b < T_{-b}\}$) scales like $\varepsilon^{-\frac{n}{n+1}}$.

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References

M. Abramowitz and I. A. Stegun. *Handbook of mathematical functions with formulas, graphs, and mathematical tables*, volume 55 of *National Bureau of Standards Applied Mathematics Series*. For sale by the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. (1964). MR0167642.

Y. Bakhtin. Exit asymptotics for small diffusion about an unstable equilibrium. *Stochastic Process. Appl.* **118** (5), 839–851 (2008). MR2411523.

N. Berglund. Kramers' law: Validity, derivations and generalisations. *ArXiv Mathematics e-prints* (2011). To appear in Markov Processes Relat. Fields. arXiv: 1106.5799.

N. Berglund and B. Gentz. On the noise-induced passage through an unstable periodic orbit. I. Two-level model. *J. Statist. Phys.* **114** (5-6), 1577–1618 (2004). MR2039489.

A. N. Borodin and P. Salminen. *Handbook of Brownian motion—facts and formulae*. Probability and its Applications. Birkhäuser Verlag, Basel, second edition (2002). ISBN 3-7643-6705-9. MR1912205.

A. Bovier, M. Eckhoff, V. Gayrard and M. Klein. Metastability in reversible diffusion processes. I. Sharp asymptotics for capacities and exit times. *J. Eur. Math. Soc. (JEMS)* **6** (4), 399–424 (2004). MR2094397.

L. Breiman. First exit times from a square root boundary. In *Proc. Fifth Berkeley Sympos. Math. Statist. and Probability (Berkeley, Calif., 1965/66), Vol. II: Contributions to Probability Theory, Part 2*, pages 9–16. Univ. California Press, Berkeley, Calif. (1967). MR0212865.

F. Cérou, A. Guyader, T. Lelièvre and D. Pommier. A multiple replica approach to simulate reactive trajectories. *J. Chem. Phys.* **134**, 054108 (2011). DOI: 10.1063/1.3518708.

M. V. Day. Some phenomena of the characteristic boundary exit problem. In *Diffusion processes and related problems in analysis, Vol. I (Evanston, IL, 1989)*, volume 22 of *Progr. Probab.*, pages 55–71. Birkhäuser Boston, Boston, MA (1990). MR1110156.

M. V. Day. Conditional exits for small noise diffusions with characteristic boundary. *Ann. Probab.* **20** (3), 1385–1419 (1992). MR1175267.

M. V. Day. On the exit law from saddle points. *Stochastic Process. Appl.* **60** (2), 287–311 (1995). MR1376805.

W. E and E. Vanden-Eijnden. Metastability, conformation dynamics, and transition pathways in complex systems. In *Multiscale modelling and simulation*, volume 39 of *Lect. Notes Comput. Sci. Eng.*, pages 35–68. Springer, Berlin (2004). MR2089952.

M. I. Freidlin and A. D. Wentzell. *Random perturbations of dynamical systems*, volume 260 of *Grundlehren der Mathematischen Wissenschaften [Fundamental Principles of Mathematical Sciences]*. Springer-Verlag, New York, second edition (1998). ISBN 0-387-98362-7. Translated from the 1979 Russian original by Joseph Szücs. MR1652127.

I. Gyöngy and N. Krylov. Existence of strong solutions for Itô's stochastic equations via approximations. *Probab. Theory Related Fields* **105** (2), 143–158 (1996). MR1392450.

G. Hummer. From transition paths to transition states and rate coefficients. *J. Chem. Phys.* **120** (2), 516–523 (2004). DOI: 10.1063/1.1630572.

I. Karatzas and S. E. Shreve. *Brownian motion and stochastic calculus*, volume 113 of *Graduate Texts in Mathematics*. Springer-Verlag, New York, second edition (1991). ISBN 0-387-97655-8. MR1121940.

J. Lu and J. Nolen. Reactive trajectories and the transition path process. *ArXiv Mathematics e-prints* (2013). arXiv: 1303.1744.

S. Luccioli, A. Imparato, S. Mitternacht, A. Irbck and A. Torcini. Unfolding times for proteins in a force clamp. *Phys Rev E Stat Nonlin Soft Matter Phys* **81**, (1 Pt 1):010902 (2010). DOI: 10.1103/PhysRevE.81.010902.

R. S. Maier and D. L. Stein. Limiting exit location distributions in the stochastic exit problem. *SIAM J. Appl. Math.* **57** (3), 752–790 (1997). MR1450848.

J.-L. Marchand. Conditioning diffusions with respect to partial observations. *ArXiv Mathematics e-prints* (2011). arXiv: 1105.1608.

G. Menz and A. Schlichting. Spectral gap estimates at low temperature by decomposition of the energy landscape. *ArXiv Mathematics e-prints* (2012). arXiv: 1202.1510.

D. Revuz and M. Yor. *Continuous martingales and Brownian motion*, volume 293 of *Grundlehren der Mathematischen Wissenschaften [Fundamental Principles of Mathematical Sciences]*. Springer-Verlag, Berlin (1991). MR1083357.

Roberto H. Schonmann. The pattern of escape from metastability of a stochastic Ising model. *Comm. Math. Phys.* **147** (2), 231–240 (1992). MR1174411.

A. Ju. Veretennikov. Strong solutions and explicit formulas for solutions of stochastic integral equations. *Mat. Sb. (N.S.)* **111(153)** (3), 434–452, 480 (1980). MR568986.