The Eyring–Kramers law for potentials with nonquadratic saddles

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Abstract

The Eyring–Kramers law describes the mean transition time of an overdamped Brownian particle between local minima in a potential landscape. In the weak-noise limit, the transition time is to leading order exponential in the potential difference to overcome. This exponential is corrected by a prefactor which depends on the principal curvatures of the potential at the starting minimum and at the highest saddle crossed by an optimal transition path. The Eyring–Kramers law, however, does not hold whenever one of these principal curvatures vanishes, since it would predict a vanishing or infinite transition time. We derive the correct prefactor up to multiplicative errors that tend to one in the zero-noise limit. As an illustration, we discuss the case of a symmetric pitchfork bifurcation, in which the prefactor can be expressed in terms of modified Bessel functions. The results extend work by Bovier, Eckhoff, Gayrard and Klein, who rigorously analysed the case of quadratic saddles, using methods from potential theory.

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1 Introduction

Consider the stochastic differential equation

$$dx_t = -\nabla V(x_t)\, dt + \sqrt{2\varepsilon}\, dW_t\ , \tag{1.1}$$

where $V : \mathbb{R}^d \to \mathbb{R}$ is a confining potential. The Eyring–Kramers law ([Eyr35, Kra40]) describes the expected transition time τ between potential minima in the small-noise limit $\varepsilon \to 0$. In the one-dimensional case ($d = 1$), it has the following form. Assume x and y are quadratic local minima of V, separated by a unique quadratic local maximum z. Then the expected transition time from x to y satisfies

$$\mathbb{E}^x\{\tau\} \simeq \frac{2\pi}{\sqrt{V''(x)|V''(z)|}}\, e^{[V(z)-V(x)]/\varepsilon}\ . \tag{1.2}$$

In the multidimensional case ($d \geqslant 2$), assume the local minima are separated by a unique saddle z, which is such that the Hessian $\nabla^2 V(z)$ admits a single negative eigenvalue $\lambda_1(z)$, while all other eigenvalues are strictly positive. Then the analogue of (1.2) reads

$$\mathbb{E}^x\{\tau\} \simeq \frac{2\pi}{|\lambda_1(z)|}\sqrt{\frac{\det(\nabla^2 V(z))}{\det(\nabla^2 V(z))}}\, e^{[V(z)-V(x)]/\varepsilon}\ . \tag{1.3}$$

This expression has been generalised to situations where there are several alternative saddles allowing to go from x to y, and to potentials with more than two minima.

A long time has elapsed between the first presentation of the formula (1.3) by Eyring [Eyr35] and Kramers [Kra40] and its rigorous mathematical proof (including a precise definition of what the symbol "$\simeq$" in (1.3) actually means). The exponential asymptotics were proved to be correct by Wentzell and Freidlin in the early Seventies, using the theory of large deviations [VF69, VF70, FW98]. While being very flexible, and allowing to study more general than gradient systems like (1.1), large deviations do not allow to obtain the prefactor of the transition time. An alternative approach is based on the fact that mean transition times obey certain elliptic partial differential equations, whose solutions can be approximated by WKB-theory (for a recent survey of these methods, see [Kol00]). This approach provides formal asymptotic series expansions in ε, whose justification is, however, a difficult problem of analysis. A framework for such a rigorous justification is provided by microlocal analysis, which was primarily developed by Helffer and Sjöstrand to solve quantum mechanical tunnelling problems in the semiclassical limit [HS84, HS85b, HS85a, HS85c]. Unfortunately, it turns out that when translated into terms of semiclassical analysis, the problem of proving the Eyring–Kramers formula becomes a particularly intricate one, known as "tunnelling through non-resonant wells". The first mathematically rigorous proof of (1.3) in arbitrary dimension (and its generalisations to more than two wells) was obtained by Bovier, Eckhoff, Gayrard and Klein [BEGK04], using a different approach based on potential theory and a variational principle. In [BEGK04], the Eyring–Kramers law is shown to hold with $a \simeq b$ meaning $a = b(1 + \mathcal{O}(\varepsilon^{1/2}|\log \varepsilon|))$. Finally, a full asymptotic expansion of the prefactor in powers of ε was proved to hold in [HKN04, HN05], using again analytical methods.

In this work, we are concerned with the case where the determinant of one of the Hessian matrices vanishes. In such a case, the expression (1.3) either diverges or goes to zero, which is obviously absurd. It seems reasonable (as has been pointed out, e.g., in [Ste05]) that one has to take into account higher-order terms of the Taylor expansion of the potential at the stationary points when estimating the transition time. Of course, cases with degenerate Hessian are in a sense not generic, so why should we care about this situation at all? The answer is that as soon as the potential depends on a parameter, degenerate stationary points are bound to occur, most noteably at bifurcation points, i.e., where the number of saddles varies as the parameter changes. See, for instance, [BFG07a, BFG07b] for an analysis of a naturally arising parameter-dependent system displaying a series of symmetry-breaking bifurcations. For this particular system, an analysis of the subexponential asymptotics of metastable transition times away from bifurcation values of the parameter has been initiated in [BB07].

In order to study sharp asymptotics of expected transition times, we rely on the potential-theoretic approach developed in [BEGK04, BGK05]. In particular, the expected transition time can be expressed in terms of so-called Newtonian capacities between sets, which can in turn be estimated by a variational principle involving Dirichlet forms. The main new aspect of the present work is that we estimate capacities in cases involving nonquadratic saddles.

In the non-degenerate case, saddles are easy to define: they are stationary points at which the Hessian has exactly one strictly negative eigenvalue, all other eigenvalues being strictly positive. When the determinant of the Hessian vanishes, the situation is not so simple, since the nature of the stationary point depends on higher-order terms in the Taylor expansion. We thus start, in Section 2, by defining and classifying saddles in degenerate cases. In Section 3, we estimate capacities for the most generic cases, which then allows us to derive expressions for the expected transition times. Section 4 contains the proofs of the main results.

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2 Classification of nonquadratic saddles

We consider a confining potential V, that is, a continuous function $V : \mathbb{R}^d \to \mathbb{R}$ satisfying a suitable growth condition at infinity. More precisely, we assume V has exponentially tight level sets, that is,

$$\int_{\{x\in\mathbb{R}^d\colon V(x)\geqslant a\}} \mathrm{e}^{-V(x)/\varepsilon}\,\mathrm{d}x \leqslant C(a)\,\mathrm{e}^{-a/\varepsilon} \qquad \forall a\in\mathbb{R}\ , \tag{2.1}$$

with $C(a)$ bounded above and uniform in $\varepsilon \leqslant 1$. We start by giving a topological definition of saddles, before classifying saddles for sufficiently differentiable potentials V.

2.1 Topological definition of saddles

We start by introducing the notion of a gate between two sets A and B. Roughly speaking, a *gate* is a set that cannot be avoided by those paths going from A to B which stay as low as possible in the potential landscape. *Saddles* will then be defined as particular points in gates.

It is useful to introduce some terminology and notations:

- For $x, y \in \mathbb{R}^d$, we denote by $\gamma : x \to y$ a *path* from x to y, that is, a continuous function $\gamma\colon [0,1] \to \mathbb{R}^d$ such that $\gamma(0) = x$ and $\gamma(1) = y$.
- The *communication height* between x and y is the highest potential value no path leading from x to y can avoid reaching, even when staying as low as possible, i.e.,

$$\overline{V}(x,y) = \inf_{\gamma\colon x\to y} \sup_{t\in[0,1]} V(\gamma(t))\ . \tag{2.2}$$

  Note that $\overline{V}(x,y) \geqslant V(x)\vee V(y)$, with equality holding, for instance, in cases where x and y are "on the same side of a mountain slope".
- The communication height between two sets $A, B \subset \mathbb{R}^d$ is given by

$$\overline{V}(A,B) = \inf_{x\in A, y\in B} \overline{V}(x,y)\ . \tag{2.3}$$

  We denote by $\mathcal{G}(A,B) = \{z\in\mathbb{R}^d\colon V(z) = \overline{V}(A,B)\}$ the level set of $\overline{V}(A,B)$.
- The *set of minimal paths* from A to B is

$$\mathcal{P}(A,B) = \left\{\gamma\colon x\to y \,\middle|\, x\in A, y\in B, \sup_{t\in[0,1]} V(\gamma(t)) = \overline{V}(A,B)\right\}\ . \tag{2.4}$$

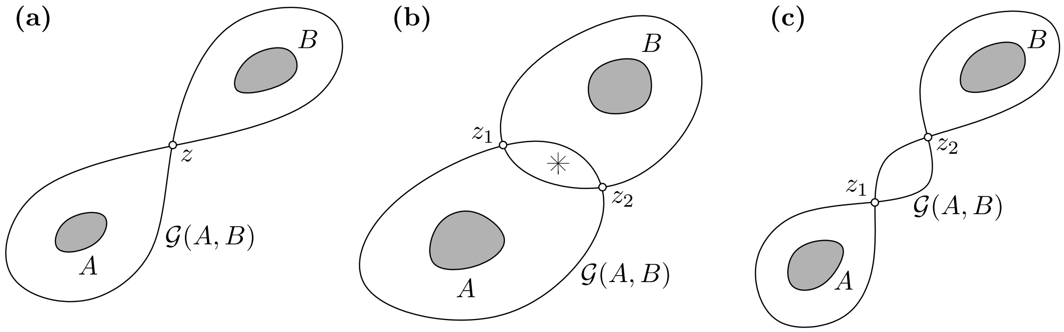

FIGURE 1. Examples of potentials and gates. **(a)** $G(A,B) = \{z\}$. **(b)** $G(A,B) = \{z_1, z_2\}$. **(c)** $G(A,B) = \{z_1\}$ or $\{z_2\}$. Here curves show level lines, shaded areas indicate potential wells and the star marks a potential maximum.

The following definition is taken from [BEGK04].

Definition 2.1. *A* gate $G(A,B)$ *is a minimal subset of* $\mathcal{G}(A,B)$ *such that all minimal paths* $\gamma \in \mathcal{P}(A,B)$ *must intersect* $G(A,B)$*.*

Let us consider some examples in dimension $d = 2$ (Figure 1):

- In uninteresting cases, e.g. for A and B on the same side of a slope, the gate $G(A,B)$ is a subset of $A \cup B$. We will not be concerned with such cases.
- If on the way from A to B, one has to cross one "mountain pass" z which is higher than all other passes, then $G(A,B) = \{z\}$ (Figure 1a).
- If there are several passes at communication height $\overline{V}(A,B)$ between A and B, between which one can choose, then the gate $G(A,B)$ is the union of these passes (Figure 1b).
- If when going from A to B, one has to cross several passes in a row, all at communication height $\overline{V}(A,B)$, then the gate $G(A,B)$ is not uniquely defined: any of the passes will form a gate (Figure 1c).
- If A and B are separated by a ridge of constant altitude $\overline{V}(A,B)$, then the whole ridge is the gate $G(A,B)$.
- If the potential contains a flat part separating A from B, at height $\overline{V}(A,B)$, then any curve in this part separating the two sets is a gate.

We now proceed to defining saddles as particular cases of isolated points in gates. However, the definition should be independent of the choice of sets A and B. In order to do this, we start by introducing notions of valleys (cf. Figure 2):

- The *closed valley* of a point $x \in \mathbb{R}^d$ is the set
$$\mathcal{CV}(x) = \left\{ y \in \mathbb{R}^d \colon \overline{V}(y,x) = V(x) \right\} . \tag{2.5}$$
It is straightforward to check that $\mathcal{CV}(x)$ is closed and path-connected.
- The *open valley* of a point $x \in \mathbb{R}^d$ is the set
$$\mathcal{OV}(x) = \left\{ y \in \mathcal{CV}(x) \colon V(y) < V(x) \right\} . \tag{2.6}$$
It is again easy to check that $\mathcal{OV}(x)$ is open. Note however that if the potential contains horizontal parts, then $\mathcal{CV}(x)$ need not be the closure of $\mathcal{OV}(x)$ (Figure 2c). Also note that $\mathcal{OV}(x)$ need not be path-connected (Figure 2b). We will use this fact to define a saddle.

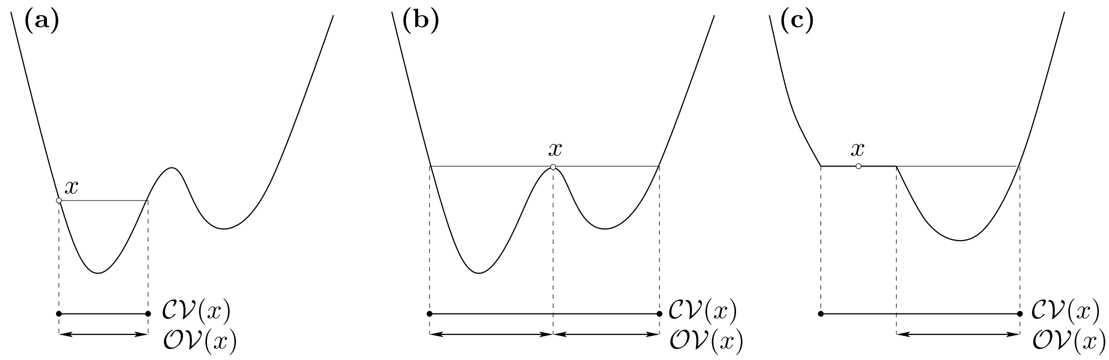

FIGURE 2. Examples of potentials and valleys. In case **(b)**, x is a saddle.

Let $\mathcal{B}_\varepsilon(x) = \{y \in \mathbb{R}^d : \|y - x\|_2 < \varepsilon\}$ denote the open ball of radius ε, centred in x.

Definition 2.2. *A* saddle *is a point $z \in \mathbb{R}^d$ such that there exists $\varepsilon > 0$ for which*

1. *$\mathcal{OV}(z) \cap \mathcal{B}_\varepsilon(z)$ is non-empty and not path-connected.*
2. *$(\mathcal{OV}(z) \cup \{z\}) \cap \mathcal{B}_\varepsilon(z)$ is path-connected.*

The link between saddles and gates is made clear by the following two results.

Proposition 2.3. *Let z be a saddle. Assume $\mathcal{OV}(z)$ is not path-connected,*[1] *and let A and B belong to different path-connected components of $\mathcal{OV}(z) \cap \mathcal{B}_\varepsilon(z)$. Then $z \in G(A, B)$.*

PROOF: Choose points $x \in A$ and $y \in B$ and a path $\gamma\colon A \to B$. Since A and B belong to different path-connected components of $\mathcal{OV}(z)$, the path γ must leave $\mathcal{OV}(z)$, which implies $\sup_{t\in[0,1]} V(\gamma(t)) \geqslant V(z)$. Since $(\mathcal{OV}(z) \cup \{z\}) \cap \mathcal{B}_\varepsilon(z)$ is path-connected, we can find a path $\gamma\colon A \to B$ staying all the time in this set, and thus for this path, $\sup_{t\in[0,1]} V(\gamma(t)) = V(z)$. As a consequence, the communication height $\overline{V}(x, y)$ equals $V(z)$, i.e., γ belongs to the set $\mathcal{P}(A, B)$ of minimal paths. Since $\mathcal{OV}(z)$ is not path-connected, we have found a path $\gamma \in \mathcal{P}(A, B)$ which must contain z, and thus $z \in G(A, B)$. □

Proposition 2.4. *Let A and B be two disjoint sets, and let $z \in G(A, B)$. Assume that z is isolated in the sense that there exists $\varepsilon > 0$ such that $\mathcal{B}^*_\varepsilon(z) := \mathcal{B}_\varepsilon(z) \setminus \{z\}$ is disjoint from the union of all gates $G(A, B)$ between A and B. Then z is a saddle.*

PROOF: Consider the set

$$D = \bigcup_{\gamma\in\mathcal{P}(A,B)} \bigcup_{t\in[0,1]} \gamma(t) \tag{2.7}$$

of all points contained in minimal paths from A to B. We claim that $D = \mathcal{CV}(z)$.

On one hand, if $x \in D$ then there exists a minimal path from A to B containing x. We follow this path backwards from x to A. Then there is a (possibly different) minimal path leading from the first path's endpoint in A through z to B. By gluing together these paths, we obtain a minimal path connecting x and z. This path never exceeds the potential value $V(z)$, which proves $\overline{V}(x, z) = V(z)$. Thus $x \in \mathcal{CV}(z)$, and $D \subset \mathcal{CV}(z)$ follows.

On the other hand, pick $y \in \mathcal{CV}(z)$. Then there is a path $\gamma_1\colon y \to z$ along which the potential does not exceed $V(z)$. Inserting this path (twice, going back and forth) in

[1]We need to make this assumption globally, in order to rule out situations where z is not the lowest saddle between two domains.

a minimal path $\gamma \in \mathcal{P}(A, B)$ containing z, we get another minimal path from A to B, containing y. This proves $y \in D$, and thus the inverse inclusion $\mathcal{CV}(z) \subset D$.

Now pick $x \in A$ and $y \in B$. There must exist a minimal path $\gamma\colon x \to y$, containing z, with the property that V is strictly smaller than $V(z)$ on $\gamma([0,1]) \cap \mathcal{B}^*_\varepsilon(z)$, since otherwise we would contradict the assumption that z be isolated. We can thus pick x' on γ between x and z and y' on γ between z and y such that $V(x') < V(z)$ and $V(y') < V(z)$. Hence we have $x', y' \in \mathcal{OV}(z)$ and any minimal path from x' to y' staying in $\mathcal{B}_\varepsilon(z)$ has to cross $z \notin \mathcal{OV}(z)$. This shows that $\mathcal{OV}(z) \cap \mathcal{B}_\varepsilon(z)$ is non-empty and not path-connected. Finally, take any $x, y \in \mathcal{OV}(z) \cap \mathcal{B}_\varepsilon(z) \subset D$. Then we can connect them by a path $\gamma \ni z$, and making ε small enough we may assume that V is strictly smaller than $V(z)$ on $\gamma([0,1]) \cap \mathcal{B}^*_\varepsilon(z)$, i.e., $\gamma([0,1]) \setminus \{z\} \subset \mathcal{OV}(z)$. This proves that $(\mathcal{OV}(z) \cup \{z\}) \cap \mathcal{B}_\varepsilon(z)$ is path-connected. □

2.2 Classification of saddles for differentiable potentials

Let us show that for sufficiently smooth potentials, our definition of saddles is consistent with the usual definition of nondegenerate saddles. Then we will start classifying degenerate saddles.

Proposition 2.5. *Let V be of class $\mathcal{C}^1$, and let z be a saddle. Then z is a stationary point of V, i.e., $\nabla V(z) = 0$.*

PROOF: Suppose, to the contrary, that $\nabla V(z) \neq 0$. We may assume $z = 0$ and $V(z) = 0$. Choose local coordinates in which $\nabla V(0) = (a, 0, \dots, 0)$ with $a > 0$. By the implicit-function theorem, there exists a differentiable function $h : \mathbb{R}^{d-1} \to \mathbb{R}^d$ such that all solutions of the equation $V(x) = 0$ in a small ball $\mathcal{B}_\varepsilon(0)$ are of the form $x_1 = h(x_2, \dots, x_d)$. Furthermore, $V(\varepsilon, 0, \dots, 0) = a\varepsilon + \mathcal{O}(\varepsilon)$ is positive for $\varepsilon > 0$ and negative for $\varepsilon < 0$. By continuity, $V(x)$ is positive for $x_1 > h(x_2, \dots, x_d)$ and negative for $x_1 < h(x_2, \dots, x_d)$, showing that $\mathcal{OV}(z) \cap \mathcal{B}_\varepsilon(0)$ is path-connected. Hence z is not a saddle. □

Proposition 2.6. *Assume V is of class $\mathcal{C}^2$, and let z be a saddle. Then*

1. *$\nabla^2 V(z)$ has at least one eigenvalue smaller or equal than 0.*
2. *$\nabla^2 V(z)$ has at most one eigenvalue strictly smaller than 0.*

PROOF: Denote the eigenvalues of $\nabla^2 V(z)$ by $\lambda_1 \leqslant \lambda_2 \leqslant \dots \leqslant \lambda_d$. We may again assume that $z = 0$ and $V(0) = 0$, and choose a basis in which the Hessian is diagonal. Then

$$V(x) = \frac{1}{2} \sum_{i=1}^{d} \lambda_i x_i^2 + \mathcal{O}(\|x\|_2^2) . \tag{2.8}$$

1. Assume, to the contrary that $\lambda_1 > 0$. Then $V > 0$ near $z = 0$, so that $\mathcal{OV}(z) = \emptyset$, and $z = 0$ is not a saddle.
2. Suppose, to the contrary, that $\lambda_1 \leqslant \lambda_2 < 0$, and fix a small $\delta > 0$. Since

$$V(x) = -\frac{1}{2}|\lambda_1| x_1^2 - \frac{1}{2}|\lambda_2| x_2^2 + \frac{1}{2} \sum_{i=3}^{d} \lambda_i x_i^2 + \mathcal{O}(\|x\|_2^2) , \tag{2.9}$$

we can find an $\varepsilon = \varepsilon(\delta) \in (0, \delta)$ such that for any fixed $(x_3, \dots, x_d)$ of length less than ε, the set $\{(x_1, x_2)\colon x_1^2 + x_2^2 < \delta^2, V(x) < 0\}$ is path-connected (topologically, it is an annulus). This implies that $\{(x_1, \dots, x_d)\colon x_1^2 + x_2^2 < \delta^2, V(x) < 0, \|(x_3, \dots, x_d)\|_2 < \varepsilon\}$ is also path-connected. Hence $\mathcal{OV}(z) \cap \mathcal{B}_\varepsilon(z)$ is path-connected. □

Proposition 2.7. *Assume V is of class $\mathcal{C}^2$, and let z be a nondegenerate stationary point, i.e. such that* $\det(\nabla^2 V(z)) \neq 0$. *Then z is a saddle if and only if $\nabla^2 V(z)$ has exactly one strictly negative eigenvalue.*

PROOF: Denote the eigenvalues of $\nabla^2 V(z)$ by $\lambda_1 \leqslant \lambda_2 \leqslant \dots \leqslant \lambda_d$. If z is a saddle, then the previous result implies that $\lambda_1 < 0 < \lambda_2$. Conversely, if $\lambda_1 < 0 < \lambda_2$, we have

$$V(x) = -\frac{1}{2}|\lambda_1| x_1^2 + \frac{1}{2}\sum_{i=2}^{d} \lambda_i x_i^2 + \mathcal{O}(\|x\|_2^2) . \tag{2.10}$$

Thus for fixed small $(x_2, \dots, x_d)$, the set $\{x_1 \colon |x_1| < \varepsilon, V(x) < 0\}$ is not path-connected, as it does not contain 0. Thus $\mathcal{OV}(z) \cap \mathcal{B}_\varepsilon(z)$ is not path-connected (it is topologically the interior of a double cone). However, for $x_1 = 0$, adding the origin makes the set path-connected, so that $(\mathcal{OV}(z) \cap \mathcal{B}_\varepsilon(z)) \cup \{z\}$ is path-connected. □

We can now classify all candidates for saddles in the following way. Let $\lambda_1 \leqslant \lambda_2 \leqslant \dots \leqslant \lambda_d$ be the eigenvalues of the Hessian $\nabla^2 V(z)$ of a stationary point z, arranged in increasing order. Then the following cases may occur:

1. $\lambda_1 < 0$:
   (a) $\lambda_2 > 0$: z is a nondegenerate saddle.
   (b) $\lambda_2 = 0$:
      i. $\lambda_3 > 0$: z is a singularity of codimension 1.
      ii. $\lambda_3 = 0$:
         A. $\lambda_4 > 0$: z is a singularity of codimension 2.
         B. $\lambda_4 = 0$: z is a singularity of codimension larger than 2.
2. $\lambda_1 = 0$:
   (a) $\lambda_2 > 0$: z is a singularity of codimension 1.
   (b) $\lambda_2 = 0$:
      i. $\lambda_3 > 0$: z is a singularity of codimension 2.
      ii. $\lambda_3 = 0$: z is a singularity of codimension larger than 2.

One can of course push further the classification, including all singularities up to codimension d. In the sequel, we shall concentrate on codimension 1.

2.3 Singularities of codimension 1

We assume in this subsection that z is a saddle point of the potential with the Hessian $\nabla^2 V(z)$ having one vanishing eigenvalue. We may assume $z = 0$ and $V(z) = 0$. According to Proposition 2.6, there are two cases to be considered:

1. $\lambda_1 < 0$, $\lambda_2 = 0$ and $0 < \lambda_3 \leqslant \dots \leqslant \lambda_d$.
2. $\lambda_1 = 0$ and $0 < \lambda_2 \leqslant \dots \leqslant \lambda_d$.

In this section, it will be convenient to relabel the first two eigenvalues in such a way that $\lambda_1 = 0$, while $\lambda_2 \neq 0$ can be positive or negative. We choose a basis in which $\nabla^2 V(z) = \operatorname{diag}(0, \lambda_2, \dots, \lambda_d)$. We shall assume that the potential V is of class $\mathcal{C}^4$, and set, for $i_1, \dots, i_p \in \{1, \dots, d\}$,

$$V_{i_1 \dots i_p} = \frac{1}{n_1! \dots n_d!} \frac{\partial}{\partial x_{i_1}} \dots \frac{\partial}{\partial x_{i_p}} V(z) , \qquad n_j = \#\{k \colon i_k = j\} , \tag{2.11}$$

with the convention that the i_k's are always in increasing order. The potential thus admits a Taylor expansion of the form

$$V(x) = \frac{1}{2}\sum_{i=2}^{d}\lambda_i x_i^2 + \sum_{1\leqslant i\leqslant j\leqslant k\leqslant d} V_{ijk}x_ix_jx_k + \sum_{1\leqslant i\leqslant j\leqslant k\leqslant l\leqslant d} V_{ijkl}x_ix_jx_kx_l + \mathcal{O}(\|x\|_2^4)\ . \quad (2.12)$$

The theory of normal forms allows to simplify this expression by constructing a change of variables $x = y + g(y)$, with g a polynomial function, such that the potential expressed in the new variables has as few as possible terms of low order in its Taylor expansion. In general, only a few so-called resonant terms cannot be eliminated, and are thus essential to describe the local dynamics.

Proposition 2.8. *There exists a polynomial change of variables $x = y + g(y)$, where g is a polynomial with terms of degree 2 and 3, such that*

$$V(y+g(y)) = \frac{1}{2}\sum_{i=2}^{d}\lambda_i y_i^2 + C_3y_1^3 + C_4y_1^4 + \mathcal{O}(\|y\|_2^4)\ , \quad (2.13)$$

where

$$C_3 = V_{111}\ , \qquad C_4 = V_{1111} - \frac{1}{2}\sum_{j=2}^{d}\frac{V_{11j}^2}{\lambda_j}\ . \quad (2.14)$$

The proof uses standard normal form theory. We give it in Appendix A. Let us now apply the result to derive an easy to verify necessary condition for a point z to be a saddle.

Corollary 2.9.

1. *Assume $\lambda_2 < 0$. Then the point z is*
   - *a saddle if $C_3 = 0$ and $C_4 > 0$;*
   - *not a saddle if $C_3 \neq 0$ or $C_4 < 0$.*
2. *Assume $\lambda_2 > 0$. Then the point z is*
   - *a saddle if $C_3 = 0$ and $C_4 < 0$;*
   - *not a saddle if $C_3 \neq 0$ or $C_4 > 0$.*

PROOF: Consider first the case $C_3 \neq 0$. For simplicity, let us restrict to $d = 2$. In a neighbourhood of $z = 0$, any solution to the equation $V(y) = 0$ must satisfy

$$y_2^2 = -\frac{2C_3}{\lambda_2}y_1^3 - \frac{2C_4}{\lambda_2}y_1^4 + \mathcal{O}(\|y\|_2^4)\ . \quad (2.15)$$

Thus, solutions exist for y_1 with $y_1C_3/\lambda_2 < 0$. Plugging the ansatz

$$y_2 = \pm\sqrt{-\frac{2C_3}{\lambda_2}y_1^3}\,\big[1 + r_2(y_1)\big] \quad (2.16)$$

into the relation $V(y) = 0$, dividing by y_1^3 and applying the implicit-function theorem to the pair (r_2, y_1) in the resulting equation shows that there is a unique curve through the origin on which the potential vanishes. Since for $y_2 = 0$, the potential has the same sign as y_1, we conclude that 0 is not a saddle. Now just note that the proof is similar in dimension $d > 2$.

Consider next the case $C_3 = 0$ and $\lambda_2 C_4 > 0$. If $\lambda_2 > 0$, one sees that the origin is a local minimum. If $\lambda_2 < 0$, then for fixed $(y_3, \dots, y_d)$ and sufficiently small ε, the set $\{(y_1, y_2) \colon y_1^2 + y_2^2 < \varepsilon^2, V(y) < 0\}$ is path-connected (topologically, it is an annulus). Hence $\mathcal{OV}(0) \cup \mathcal{B}_\varepsilon(0)$ is path-connected.

Finally, if $C_3 = 0$ and $\lambda_2 C_4 > 0$, then either the set $\{y_1 \colon V(y) < 0\}$ for fixed $(y_2, \dots, y_d)$ or the set $\{y_2 \colon V(y) < 0\}$ for fixed $(y_1, y_3, \dots, y_d)$ is not path-connected, so that the valley of 0 is locally split into two disconnected components, joined at the origin. □

Remark 2.10. The normal-form transformation $x \mapsto x + g(x)$ can also be applied when $\lambda_1 \neq 0$. The result is exactly the same normal form as in (2.13), except that there is an additional term $\frac{1}{2}\lambda_1 y_1^2$. This is useful as it allows to study the system with a unique transformation of variables in a full neighbourhood of the bifurcation point.

Remark 2.11. One easily checks that if V is of class $\mathcal{C}^p$, one can construct higher-order normal forms by eliminating all terms which are not of the form y_1^k for some $k \leqslant p$. In other words, there exists a polynomial $g(y)$ such that

$$V(y + g(y)) = \frac{1}{2}\sum_{i=2}^{d} \lambda_i y_i^2 + C_3 y_1^3 + C_4 y_1^4 + \dots + C_p y_1^p + \mathcal{O}(\|y\|_2^p) \,. \tag{2.17}$$

In general, however, there is no simple expression of the coefficients of the normal form in terms of the original Taylor coefficients of V.

3 First-passage times for nonquadratic saddles

3.1 Some potential theory

Let $(x_t)_t$ be the solution of the stochastic differential equation (1.1). Given a measurable set $A \subset \mathbb{R}^d$, we denote by $\tau_A = \inf\{t > 0 \colon x_t \in A\}$ the first-hitting time of A. For sets[2] $A, B \subset \mathbb{R}^d$, the quantity

$$h_{A,B}(x) = \mathbb{P}^x\bigl\{\tau_A < \tau_B\bigr\} \tag{3.1}$$

is known to satisfy the boundary value problem

$$\begin{cases} Lh_{A,B}(x) = 0 & \text{for } x \in (A \cup B)^c \,, \\ h_{A,B}(x) = 1 & \text{for } x \in A \,, \\ h_{A,B}(x) = 0 & \text{for } x \in B \,, \end{cases} \tag{3.2}$$

where $L = \varepsilon\Delta - \langle\nabla V(\cdot), \nabla\rangle$ is the infinitesimal generator of the diffusion $(x_t)_t$. By analogy with the electrical potential created between two conductors at potentials respectively 1 and 0, $h_{A,B}$ is called the *equilibrium potential* of A and B. More generally, one can define an equilibrium potential $h^\lambda_{A,B}$, defined by a similar boundary value problem as (3.2), but with $Lh^\lambda_{A,B} = \lambda h^\lambda_{A,B}$. However, we will not need this generalisation here.

The *capacity* of the sets A and B is again defined in analogy with electrostatics as the total charge accumulated on one conductor of a capacitor, for unit potential difference. The most useful expression for our purpose is the integral, or *Dirichlet form*

$$\operatorname{cap}_A(B) = \varepsilon \int_{(A\cup B)^c} \mathrm{e}^{-V(x)/\varepsilon} \|\nabla h_{A,B}(x)\|_2^2 \, \mathrm{d}x =: \Phi_{(A\cup B)^c}(h_{A,B}) \,. \tag{3.3}$$

[2]All subsets of $\mathbb{R}^d$ we consider from now on will be assumed to be *regular*, that is, such that their complement is a region with continuously differentiable boundary.

We will use the fact that the equilibrium potential $h_{A,B}$ minimizes the Dirichlet form $\Phi_{(A\cup B)^c}$, i.e.

$$\operatorname{cap}_A(B) = \inf_{h\in\mathcal{H}_{A,B}} \Phi_{(A\cup B)^c}(h) \;. \tag{3.4}$$

Here $\mathcal{H}_{A,B}$ is the space of twice weakly differentiable functions, whose derivatives up to order 2 are in L^2, and which satisfy the boundary conditions in (3.2).

Proposition 6.1 in [BEGK04] shows (under some assumptions which can be relaxed to suit our situation) that if x is a (quadratic) local minimum of the potential, then the expected first-hitting time of a set B is given by

$$\mathbb{E}^x\{\tau_B\} = \frac{\displaystyle\int_{B^c} \mathrm{e}^{-V(y)/\varepsilon}\, h_{\mathcal{B}_\varepsilon(x),B}(y)\;\mathrm{d}y}{\operatorname{cap}_{\mathcal{B}_\varepsilon(x)}(B)} \;. \tag{3.5}$$

The numerator can be estimated by the Laplace method, using some rough a priori estimates on the equilibrium potential $h_{\mathcal{B}_\varepsilon(x),B}$. In the generic situation where x is a quadratic local minimum, and the saddle z forms the gate from x to B, it is known that

$$\int_{B^c} \mathrm{e}^{-V(y)/\varepsilon}\, h_{\mathcal{B}_\varepsilon(x),B}(y)\;\mathrm{d}y = \frac{(2\pi\varepsilon)^{d/2}}{\sqrt{\det(\nabla^2 V(x))}}\,\mathrm{e}^{-V(x)/\varepsilon}\bigl[1+\mathcal{O}(\varepsilon^{1/2}|\log\varepsilon|)\bigr] \;, \tag{3.6}$$

cf. [BEGK04, Equation (6.13)]. The crucial quantity to be computed is the capacity in the denominator. In the simplest case of a quadratic saddle z whose Hessian has eigenvalues $\lambda_1 < 0 < \lambda_2 \leqslant \dots \leqslant \lambda_d$, one finds

$$\operatorname{cap}_{\mathcal{B}_\varepsilon(x)}(B) = \frac{1}{2\pi}\sqrt{\frac{(2\pi\varepsilon)^d|\lambda_1|}{\lambda_2\dots\lambda_d}}\,\mathrm{e}^{-V(z)/\varepsilon}\bigl[1+\mathcal{O}(\varepsilon^{1/2}|\log\varepsilon|)\bigr] \;, \tag{3.7}$$

cf. [BEGK04, Theorem 5.1], which implies the standard Eyring–Kramers formula (1.3).

3.2 Capacities and transition times for nonquadratic saddles

We assume in this section that the potential is of class $\mathcal{C}^5$ at least, as this allows a better control of the error terms. Consider first the case of a saddle z such that the Hessian matrix $\nabla^2 V(z)$ has eigenvalues $\lambda_1 = 0 < \lambda_2 \leqslant \lambda_3 \leqslant \dots \leqslant \lambda_d$. According to Corollary 2.9, in the most generic case the potential admits a normal form

$$V(y) = -C_4 y_1^4 + \frac12 \sum_{j=2}^d \lambda_j y_j^2 + \mathcal{O}(\|y\|_2^5) \tag{3.8}$$

with $C_4 > 0$. (Note that the saddle z is at the origin 0 of this coordinate system.)

We are interested in transition times between sets A and B for which the gate $G(A,B)$ consists only of the saddle z. In other words, we assume that any critical path $\gamma\in\mathcal{P}(A,B)$ admits z as unique point of highest altitude. This does not exclude the existence of other, lower saddles between A and B.

Theorem 3.1. *Assume z is a saddle whose normal form satisfies* (3.8)*. Let x be a local minimum of the potential, and let B be a set such that x and B belong to different path-connected components of $\mathcal{OV}(z)$. Assume finally that $G(\{x\},B) = \{z\}$. Then*

$$\operatorname{cap}_{\mathcal{B}_\varepsilon(x)}(B) = \frac{2C_4^{1/4}}{\Gamma(1/4)}\sqrt{\frac{(2\pi)^{d-1}}{\lambda_2\dots\lambda_d}}\,\varepsilon^{d/2+1/4}\,\mathrm{e}^{-V(z)/\varepsilon}\bigl[1+\mathcal{O}(\varepsilon^{1/4}|\log\varepsilon|^{1/4})\bigr] \;, \tag{3.9}$$

where Γ denotes the Euler Gamma function.

The proof is given in Section 4.3. In the case of a quadratic local minimum x, combining this result with Estimate (3.6) immediately yields the following result on first-hitting times.

Corollary 3.2. *In the above situation, the expected first-hitting time of B satisfies*

$$\mathbb{E}^x\{\tau_B\} = \frac{\Gamma(1/4)}{2C_4^{1/4}} \sqrt{\frac{2\pi\lambda_2 \dots \lambda_d}{\det(\nabla^2 V(x))}} \varepsilon^{-1/4} \, \mathrm{e}^{[V(z)-V(x)]/\varepsilon} \big[1 + \mathcal{O}(\varepsilon^{1/4} |\log \varepsilon|^{1/4})\big] . \qquad (3.10)$$

Note in particular that unlike in the quadratic case, the subexponential asymptotics depends on ε to leading order, namely proportionally to $\varepsilon^{-1/4}$.

Remark 3.3.

1. If the gate $G(\{x\}, B)$ contains several isolated saddles, the capacity is obtained simply by adding the contributions of each individual saddle. In other words, just as in electrostatics, for capacitors in parallel the equivalent capacity is obtained by adding the capacities of individual capacitors.
2. Assume the potential V is of class $2p+1$ for some $p \geqslant 2$, and that the normal form at the origin reads

$$V(y) = -C_{2p} y_1^{2p} + \frac{1}{2} \sum_{j=2}^{d} \lambda_j y_j^2 + \mathcal{O}(\|y\|_2^{2p+1}) . \qquad (3.11)$$

   Then a completely analogous proof shows that (3.9) is to be replaced by

$$\operatorname{cap}_{\mathcal{B}_\varepsilon(x)}(B) = \frac{p C_{2p}^{1/2p}}{\Gamma(1/2p)} \sqrt{\frac{(2\pi)^{d-1}}{\lambda_2 \dots \lambda_d}} \, \varepsilon^{d/2+(p-1)/2p} \big[1 + \mathcal{O}(\varepsilon^{1/2p} |\log \varepsilon|^{1/2p})\big] . \qquad (3.12)$$

   As a consequence, the subexponential prefactor of the expected first-hitting time behaves like $\varepsilon^{-(p-1)/2p}$.

Consider next the case of a saddle z such that the Hessian matrix $\nabla^2 V(x)$ has eigenvalues $\lambda_1 < \lambda_2 = 0 < \lambda_3 \leqslant \dots \leqslant \lambda_d$. Still according to Corollary 2.9, in the most generic case the potential admits a normal form

$$V(y) = -\frac{1}{2}|\lambda_1| y_1^2 + C_4 y_2^4 + \frac{1}{2} \sum_{j=3}^{d} \lambda_j y_j^2 + \mathcal{O}(\|y\|_2^5) \qquad (3.13)$$

with $C_4 > 0$.

Theorem 3.4. *Assume z is a saddle whose normal form satisfies* (3.13)*. Let x be a local minimum of the potential, and let B be a set such that x and B belong to different path-connected components of $\mathcal{OV}(z)$. Assume finally that $G(\{x\}, B) = \{z\}$. Then*

$$\operatorname{cap}_{\mathcal{B}_\varepsilon(x)}(B) = \frac{\Gamma(1/4)}{2C_4^{1/4}} \sqrt{\frac{(2\pi)^{d-3}|\lambda_1|}{\lambda_3 \dots \lambda_d}} \, \varepsilon^{d/2-1/4} \, \mathrm{e}^{-V(z)/\varepsilon} \big[1 + \mathcal{O}(\varepsilon^{1/4} |\log \varepsilon|^{1/4})\big] . \qquad (3.14)$$

The proof is given in Section 4.3. In the case of a quadratic local minimum x, combining this result with Estimate (3.6) immediately yields the following result on first-hitting times.

Corollary 3.5. *In the above situation, the expected first-hitting time of B satisfies*

$$\mathbb{E}^x\{\tau_B\} = \frac{2C_4^{1/4}}{\Gamma(1/4)} \sqrt{\frac{(2\pi)^3 \lambda_3 \dots \lambda_d}{|\lambda_1| \det(\nabla^2 V(x))}} \varepsilon^{1/4} \, \mathrm{e}^{[V(z)-V(x)]/\varepsilon} \big[1 + \mathcal{O}(\varepsilon^{1/4} |\log \varepsilon|^{1/4})\big] . \qquad (3.15)$$

Note again the ε-dependence of the prefactor, which is now proportional to $\varepsilon^{1/4}$ to leading order. A similar result is easily obtained in the case of the leading term in the normal form having order y_2^{2p} for some $p \geqslant 2$. In particular, the prefactor of the transition time then has leading order $\varepsilon^{1/2p}$.

3.3 Symmetric pitchfork bifurcation

While the results in the previous section describe the situation with nonquadratic saddles, that is, at a bifurcation point, they do not incorporate the transition from quadratic to nonquadratic saddles. In order to complete the picture, we now give a description of the metastable timescale in a full neighbourhood of a bifurcation point.

Let us assume that the potential V depends continuously on a parameter γ. For $\gamma = \gamma^\star$, $z = 0$ is a nonquadratic saddle of V, with normal form (3.13). A symmetric pitchfork bifurcation occurs when for γ near $\gamma^\star$, the normal form has the expression

$$V(y) = \frac{1}{2}\lambda_1(\gamma)y_1^2 + \frac{1}{2}\lambda_2(\gamma)y_2^2 + C_4(\gamma)y_2^4 + \frac{1}{2}\sum_{j=3}^{d}\lambda_j(\gamma)y_j^2 + \mathcal{O}(\|y\|_2^5) , \tag{3.16}$$

where $\lambda_2(\gamma^\star) = 0$, while $\lambda_1(\gamma^\star) = \lambda_1 < 0$, $C_4(\gamma^\star) = C_4 > 0$, and similarly for the other quantities. We assume here that V is even in y_2, which is the most common situation in which pitchfork bifurcations are observed. For simplicity, we shall usually refrain from indicating the γ-dependence of the eigenvalues in the sequel. All quantities except λ_2 are assumed to be bounded away from zero.

When $\lambda_2 > 0$, $z = 0$ is a quadratic saddle. When $\lambda_2 < 0$, $z = 0$ is no longer a saddle (the origin then having a two-dimensional unstable manifold), but there exist two saddles $z_\pm$ with coordinates

$$z_\pm = \bigl(0, \pm\bigl[\sqrt{|\lambda_2|/4C_4} + \mathcal{O}(\lambda_2)\bigr], 0, \dots, 0\bigr) . \tag{3.17}$$

Let us denote the eigenvalues of $\nabla^2 V(z_\pm)$ by $\mu_1, \dots, \mu_d$. In fact, for $\lambda_2 < 0$ we have

$$\begin{aligned} \mu_2 &= -2\lambda_2 + \mathcal{O}(|\lambda_2|^{3/2}) , \\ \mu_j &= \lambda_j + \mathcal{O}(|\lambda_2|^{3/2}) \qquad\qquad \text{for } j \in \{1, 3, \dots, d\} . \end{aligned} \tag{3.18}$$

Finally, the value of the potential on the saddles $z_\pm$ satisfies

$$V(z_+) = V(z_-) = V(z) - \frac{\lambda_2^2}{16C_4} + \mathcal{O}(|\lambda_2|^{5/2}) . \tag{3.19}$$

Example 3.6. In [BFG07a], we studied the potential landscape of a system of N particles on a circle, where each particle interacts with its nearest neighbours through a quadratic potential, and with an on-site double-well potential $U(x) = \frac{1}{4}x^4 - \frac{1}{2}x^2$. For $N = 2$ particles, the potential reads

$$V(x_1, x_2) = U(x_1) + U(x_2) + \frac{\gamma}{2}(x_1 - x_2)^2 . \tag{3.20}$$

Performing a rotation by $\pi/4$ yields the equivalent potential

$$\widehat{V}(y_1, y_2) = -\frac{1}{2}y_1^2 - \frac{1 - 2\gamma}{2}y_2^2 + \frac{1}{8}(y_1^4 + 6y_1^2y_2^2 + y_2^4) , \tag{3.21}$$

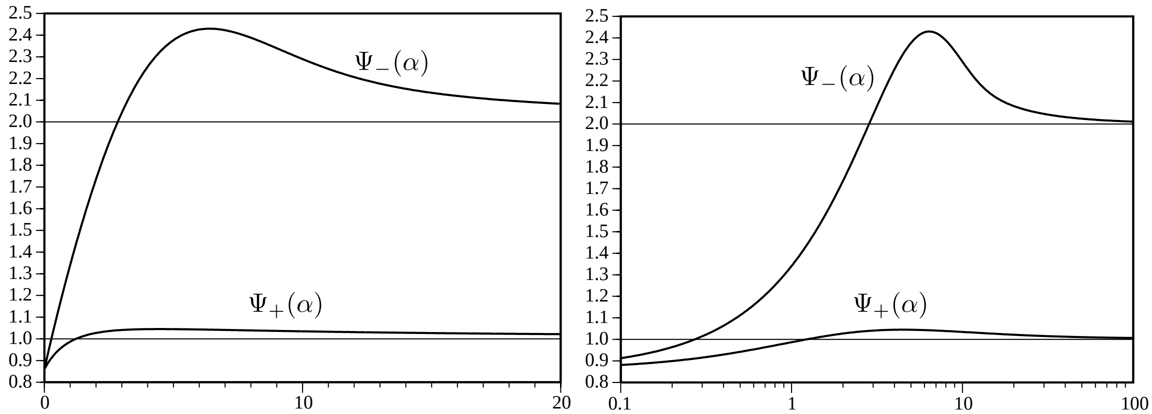

FIGURE 3. The functions $\Psi_\pm(\alpha)$, shown on a linear and on a logarithmic scale.

which immediately shows that the origin $(0,0)$ is a stationary point with $\lambda_1(\gamma) = -1/2$ and $\lambda_2(\gamma) = -(1-2\gamma)$. For $\gamma > \gamma^\star = 1/2$, the origin is thus a quadratic saddle, at altitude 0. It serves as a gate between the local minima located at $y = (\pm 1/\sqrt{2}, 0)$. As γ decreases below $\gamma^\star$, two new saddles appear at $y = (0, \pm\sqrt{2(1-2\gamma)})$. They have a positive eigenvalue $\mu_2(\gamma) = 2(2\gamma - 1)$, and the altitude $-\frac{1}{2}(1-2\gamma)^2$. There is thus a pitchfork bifurcation at $\gamma = 1/2$. Note that another pitchfork bifurcation occurs at $\gamma = 1/3$.

Our main result is the following sharp estimate of the capacity.

Theorem 3.7. *Assume z is a saddle whose normal form satisfies (3.16). Let x be a local minimum of the potential, and let B be a set such that x and B belong to different path-connected components of $\mathcal{OV}(z)$ (respectively of $\mathcal{OV}(z_\pm)$ if $\lambda_2 < 0$). Assume further that $G(\{x\}, B) = \{z\}$ (resp. $G(\{x\}, B) = \{z_-, z_+\}$ if $\lambda_2 < 0$). Then for $\lambda_2 > 0$,*

$$\operatorname{cap}_{\mathcal{B}_\varepsilon(x)}(B) = \sqrt{\frac{(2\pi)^{d-2}|\lambda_1|}{[\lambda_2 + (2C_4\varepsilon)^{1/2}]\lambda_3 \dots \lambda_d}}\,\Psi_+\biggl(\frac{\lambda_2}{\sqrt{2\varepsilon C_4}}\biggr)\varepsilon^{d/2}\,\mathrm{e}^{-V(z)/\varepsilon}\bigl[1 + R_+(\varepsilon, \lambda_2)\bigr]\;, \tag{3.22}$$

while for $\lambda_2 < 0$,

$$\operatorname{cap}_{\mathcal{B}_\varepsilon(x)}(B) = \sqrt{\frac{(2\pi)^{d-2}|\mu_1|}{[\mu_2 + (2C_4\varepsilon)^{1/2}]\mu_3 \dots \mu_d}}\,\Psi_-\biggl(\frac{\mu_2}{\sqrt{2\varepsilon C_4}}\biggr)\varepsilon^{d/2}\,\mathrm{e}^{-V(z_\pm)/\varepsilon}\bigl[1 + R_-(\varepsilon, \mu_2)\bigr]\;. \tag{3.23}$$

The functions Ψ_+ and Ψ_- are bounded above and below uniformly on $\mathbb{R}_+$. They admit the explicit expressions

$$\begin{aligned}\Psi_+(\alpha) &= \sqrt{\frac{\alpha(1+\alpha)}{8\pi}}\,\mathrm{e}^{\alpha^2/16}\,K_{1/4}\biggl(\frac{\alpha^2}{16}\biggr)\;,\\ \Psi_-(\alpha) &= \sqrt{\frac{\pi\alpha(1+\alpha)}{32}}\,\mathrm{e}^{-\alpha^2/64}\biggl[I_{-1/4}\biggl(\frac{\alpha^2}{64}\biggr) + I_{1/4}\biggl(\frac{\alpha^2}{64}\biggr)\biggr]\;,\end{aligned} \tag{3.24}$$

where $K_{1/4}$ and $I_{\pm 1/4}$ denote modified Bessel functions of the second and first kind, respectively. In particular,

$$\lim_{\alpha\to+\infty}\Psi_+(\alpha) = 1\;, \qquad \lim_{\alpha\to+\infty}\Psi_-(\alpha) = 2\;, \tag{3.25}$$

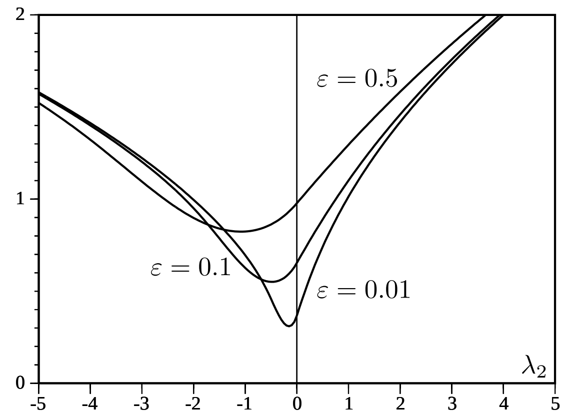

FIGURE 4. The prefactor of the expected transition time near a pitchfork bifurcation, as a function of the bifurcation parameter λ_2, shown for three different values of ε. (To be precise, we show the function $\lambda_2 \mapsto \sqrt{\lambda_2 + \varepsilon^{1/2}}/\Psi_+(\lambda_2/\varepsilon^{1/2})$ for $\lambda_2 > 0$ and the function $\lambda_2 \mapsto \sqrt{-2\lambda_2 + \varepsilon^{1/2}}/\Psi_-(-2\lambda_2/\varepsilon^{1/2})$ for $\lambda_2 < 0$.)

and

$$\lim_{\alpha\to 0} \Psi_+(\alpha) = \lim_{\alpha\to 0} \Psi_-(\alpha) = \frac{\Gamma(1/4)}{2^{5/4}\sqrt{\pi}} \simeq 0.8600 \,. \tag{3.26}$$

Finally, the error terms satisfy

$$\bigl|R_\pm(\varepsilon,\lambda)\bigr| \leqslant C\biggl[\frac{\varepsilon|\log\varepsilon|}{\bigl[|\lambda| \vee (\varepsilon|\log\varepsilon|)^{1/2}\bigr]}\biggr]^{1/2} \,. \tag{3.27}$$

The functions $\Psi_\pm(\alpha)$ are shown in Figure 3. Note in particular that they are not monotonous, but both admit a maximum.

Corollary 3.8. *In the above situation, the expected first-hitting time of B satisfies*

$$\mathbb{E}^x\bigl\{\tau_B\bigr\} = 2\pi\sqrt{\frac{[\lambda_2 + (2\varepsilon C_4)^{1/2}]\lambda_3\dots\lambda_d}{|\lambda_1|\det(\nabla^2 V(x))}}\,\frac{\mathrm{e}^{[V(z)-V(x)]/\varepsilon}}{\Psi_+\bigl(\lambda_2/(2\varepsilon C_4)^{1/2}\bigr)}\bigl[1 + R_+(\varepsilon,\lambda_2)\bigr] \tag{3.28}$$

for $\lambda_2 > 0$ and

$$\mathbb{E}^x\bigl\{\tau_B\bigr\} = 2\pi\sqrt{\frac{[\mu_2 + (2\varepsilon C_4)^{1/2}]\mu_3\dots\mu_d}{|\mu_1|\det(\nabla^2 V(x))}}\,\frac{\mathrm{e}^{[V(z_\pm)-V(x)]/\varepsilon}}{\Psi_-\bigl(\mu_2/(2\varepsilon C_4)^{1/2}\bigr)}\bigl[1 + R_-(\varepsilon,\mu_2)\bigr] \tag{3.29}$$

for $\lambda_2 < 0$.

When λ_2 is bounded away from zero, the expression (3.28) reduces to the usual Eyring–Kramers formula (1.3). When $\lambda_2 \to 0$, it converges to the limiting expression (3.15). The function Ψ_+ controls the crossover between the two regimes, which takes place when λ_2 is of order $\varepsilon^{1/2}$. In fact, when $\lambda_2 \ll \varepsilon^{1/2}$, there is a saturation effect, in the sense that the system behaves as if the curvature of the potential were bounded below by $(2\varepsilon C_4)^{1/2}$. Similar remarks apply to the expression (3.29), the only difference being a factor 1/2 in the prefactor when μ_2 is bounded away from 0 (cf. (3.25)), which is due to the fact that the gate between x and B then contains two saddles.

The λ_2-dependence of the prefactor is shown in Figure 4. It results from the combined effect of the term under the square root and the factors $\Psi_\pm$. Note in particular that the minimal value of the prefactor is located at a negative value of λ_2, which can be shown to be of order $\varepsilon^{1/2}$.

4 Proofs

4.1 Upper bound

We assume that the potential V is of class $\mathcal{C}^{2r+1}$ for some $r \geqslant 2$, and that the origin 0 is a saddle with eigenvalues satisfying $\lambda_1 \leqslant 0 \leqslant \lambda_2 < \lambda_3 \leqslant \dots \leqslant \lambda_d$. In the vicinity of the origin, V admits a normal form

$$V(y) = -u_1(y_1) + u_2(y_2) + \frac{1}{2}\sum_{j=3}^{d} \lambda_j y_j^2 + \mathcal{O}(\|y\|_2^{2r+1}) \,, \tag{4.1}$$

where we may assume that

- $u_1(y_1) = \sum_{j=2}^{2p} a_j y_1^j$ for some $1 \leqslant p \leqslant r$, with $a_{2p} > 0$;
- $u_2(y_2) = \sum_{j=2}^{2q} b_j y_2^j$ for some $1 \leqslant q \leqslant r$, with $b_{2q} > 0$.

Note that for bifurcations with a single zero eigenvalue, as considered here, either $p = 1$ (and thus $q = r$), or $q = 1$ (and thus $p = r$).

Let A and B belong to two different path-connected components of $\mathcal{OV}(0)$. We assume for simplicity that the gate $G(A, B)$ consists of the origin 0 only. However, the results can easily be extended to situations with several gates, simply by summing the contributions of all gates.

Proposition 4.1 (Upper bound)**.** *Assume there exist strictly positive numbers $\delta_1 = \delta_1(\varepsilon)$, $\delta_2 = \delta_2(\varepsilon)$ and c (independent of ε) such that*

$$\begin{aligned}
u_1(y_1) &\leqslant d\varepsilon|\log\varepsilon| && \text{whenever } |y_1| \leqslant \delta_1 \,, \\
u_2(y_2) &\geqslant -cd\varepsilon|\log\varepsilon| && \text{whenever } |y_2| \leqslant \delta_2 \,, \\
u_2(y_2) &\geqslant 2d\varepsilon|\log\varepsilon| && \text{whenever } |y_2| \geqslant \delta_2 \,,
\end{aligned} \tag{4.2}$$

and such that

$$\bigl[\delta_1(\varepsilon) + \delta_2(\varepsilon)\bigr]^{2r+1} = \mathcal{O}(\varepsilon|\log\varepsilon|) \,. \tag{4.3}$$

Then

$$\operatorname{cap}_A(B) \leqslant \varepsilon \frac{\displaystyle\int_{-\delta_2}^{\delta_2} \mathrm{e}^{-u_2(y_2)/\varepsilon} \,\mathrm{d}y_2}{\displaystyle\int_{-\delta_1}^{\delta_1} \mathrm{e}^{-u_1(y_1)/\varepsilon} \,\mathrm{d}y_1} \prod_{j=3}^{d} \sqrt{\frac{2\pi\varepsilon}{\lambda_j}} \bigl[1 + R_1(\varepsilon)\bigr] + R_2(\varepsilon) \,, \tag{4.4}$$

where the error terms satisfy

$$\begin{aligned}
R_1(\varepsilon) &\leqslant C\bigl[\varepsilon^{r-1/2}|\log\varepsilon|^{r+1/2} + \varepsilon^{-1}(\delta_1^{2r+1} + \delta_2^{2r+1}) + \delta_1 + \delta_2\bigr] \\
R_2(\varepsilon) &\leqslant C\varepsilon^{d/2+(r-1/2)/(r+1/2)}
\end{aligned} \tag{4.5}$$

for some constant $C > 0$.

Proof: The proof is adapted from the proof of [BEGK04, Theorem 5.1].

Recall that the capacity is computed as the minimal value of the Dirichlet form $\Phi_{(A\cup B)^c}$, cf. (3.4), which involves an integration over x. In the vicinity of the saddle, we carry out the normal-form transformation of Proposition 2.8 in the integral. This can always be made locally, setting $x = y + \rho \circ g(y)$, where ρ is a smooth cut-off function which is the identity in a small ball of radius Δ, and identically zero outside a larger ball of radius 2Δ.

Inside this ball, we may thus assume that the potential is given by (4.1). The Jacobian of the transformation yields a multiplicative error term $1 + \mathcal{O}(\Delta)$.

Let $\delta = 2\sqrt{(1+c)d\varepsilon|\log\varepsilon|}$. We introduce a set

$$C_\varepsilon = \prod_{j=1}^{d} [-\delta_j, \delta_j] \;, \tag{4.6}$$

where δ_1 and δ_2 satisfy (4.2) and (4.3) and we choose

$$\delta_j = \frac{\delta}{\sqrt{\lambda_j}} \;, \quad j = 3, \dots, d \;. \tag{4.7}$$

By assumption, making ε small enough we can construct a layer $\mathcal{S}_\varepsilon$ of width $2\delta_1$, separating the connected components of the open valley $\mathcal{OV}(0)$, and such that $V(y)$ is strictly positive for all $y \in \mathcal{S}_\varepsilon \setminus C_\varepsilon$. Let D_- and D_+ denote the connected components of $\mathbb{R}^d \setminus \mathcal{S}_\varepsilon$ containing A and B respectively. Then the radius Δ of the ball in which we carry out the normal form transformation can be taken as $\delta \vee \delta_1 \vee \delta_2$.

The variational principle (3.4) implies that it is sufficient to construct a function $h^+ \in \mathcal{H}_{A,B}$ such that $\Phi_{(A\cup B)^c}(h^+)$ satisfies the upper bound. We choose

$$h^+(y) = \begin{cases} 1 & \text{for } y \in D_- \;, \\ 0 & \text{for } y \in D_+ \;, \\ f(y_1) & \text{for } y \in C_\varepsilon \;, \end{cases} \tag{4.8}$$

while $h^+(y)$ is arbitrary for $y \in \mathcal{S}_\varepsilon \setminus C_\varepsilon$, except that we require $\|\nabla h^+\|_2 \leqslant \mathit{const}/\delta_1$. The function $f(y_1)$ is chosen as the solution of the one-dimensional differential equation

$$\varepsilon f''(y_1) - \frac{\partial V}{\partial y_1}(y_1, 0, \dots, 0) f'(y_1) = 0 \tag{4.9}$$

with boundary conditions 1 in $-\delta_1$ and 0 in δ_1, that is,

$$f(y_1) = \frac{\displaystyle\int_{y_1}^{\delta_1} \mathrm{e}^{V(t,0,\dots,0)/\varepsilon} \,\mathrm{d}t}{\displaystyle\int_{-\delta_1}^{\delta_1} \mathrm{e}^{V(t,0,\dots,0)/\varepsilon} \,\mathrm{d}t} \;. \tag{4.10}$$

Inserting h^+ into the expression (3.3) of the capacity, we obtain two non-vanishing terms, namely the integrals over $\mathcal{S}_\varepsilon \setminus C_\varepsilon$ and over C_ε. The first of these can be bounded as follows. For $y \in \mathcal{S}_\varepsilon \setminus C_\varepsilon$ close to the saddle, Assumptions (4.2) and (4.3) imply

$$\begin{aligned} \frac{V(y)}{\varepsilon} &\geqslant -d|\log\varepsilon| - cd|\log\varepsilon| + 2(1+c)d|\log\varepsilon| + \mathcal{O}\big(\varepsilon^{-1}\big[\delta + \delta_1 + \delta_2\big]^{2r+1}\big) \\ &\geqslant \frac{1}{2} d|\log\varepsilon| \end{aligned} \tag{4.11}$$

for sufficiently small ε. For $y \in \mathcal{S}_\varepsilon \setminus C_\varepsilon$ further away from the saddle, $V(y)$ is bounded below (and increases at infinity) by construction of $\mathcal{S}_\varepsilon$. It follows that

$$\varepsilon \int_{\mathcal{S}_\varepsilon \setminus C_\varepsilon} \mathrm{e}^{-V(y)/\varepsilon} \frac{\mathit{const}}{\delta_1^2} \,\mathrm{d}y = \mathcal{O}\big(\varepsilon^{1+d/2}\delta_1^{-2}\big) = \mathcal{O}\big(\varepsilon^{d/2+(r-1/2)/(r+1/2)}\big) =: R_2(\varepsilon) \;. \tag{4.12}$$

The second term is given by

$$\Phi_{C_\varepsilon}(h^+) = \varepsilon \int_{-\delta_d}^{\delta_d} \dots \int_{-\delta_2}^{\delta_2} \int_{-\delta_1}^{\delta_1} \mathrm{e}^{-V(y)/\varepsilon} |f'(y_1)^2| \,\mathrm{d}y_1 \,\mathrm{d}y_2 \dots \mathrm{d}y_d$$
$$= \varepsilon \frac{\displaystyle\int_{C_\varepsilon} \mathrm{e}^{-V(y)/\varepsilon} \,\mathrm{e}^{2V(y_1,0,\dots,0)/\varepsilon} \,\mathrm{d}y}{\displaystyle\biggl(\int_{-\delta_1}^{\delta_1} \mathrm{e}^{V(y_1,0,\dots,0)/\varepsilon} \,\mathrm{d}y_1\biggr)^2} . \tag{4.13}$$

By (4.1), we have for $y \in C_\varepsilon$

$$V(y) - 2V(y_1, 0, \dots, 0) = u_1(y_1) + u_2(y_2) + \frac{1}{2}\sum_{j=3}^{d} \lambda_j y_j^2 + \mathcal{O}\bigl([\delta + \delta_1 + \delta_2]^{2r+1}\bigr) . \tag{4.14}$$

Hence the numerator in (4.13) is given by

$$\int_{-\delta_1}^{\delta_1} \mathrm{e}^{-u_1(y_1)/\varepsilon} \,\mathrm{d}y_1 \int_{-\delta_2}^{\delta_2} \mathrm{e}^{-u_2(y_2)/\varepsilon} \,\mathrm{d}y_2 \prod_{j=3}^{d} \int_{-\delta_j}^{\delta_j} \mathrm{e}^{-\lambda_j y_j^2/2\varepsilon} \,\mathrm{d}y_j \biggl[1 + \mathcal{O}\biggl(\frac{[\delta + \delta_1 + \delta_2]^{2r+1}}{\varepsilon}\biggr)\biggr] . \tag{4.15}$$

Substituting in (4.13) we get

$$\Phi_{C_\varepsilon}(h^+) = \varepsilon \frac{\displaystyle\int_{-\delta_2}^{\delta_2} \mathrm{e}^{-u_2(y_2)/\varepsilon} \,\mathrm{d}y_2}{\displaystyle\int_{-\delta_1}^{\delta_1} \mathrm{e}^{-u_1(y_1)/\varepsilon} \,\mathrm{d}y_1} \prod_{j=3}^{d} \int_{-\delta_j}^{\delta_j} \mathrm{e}^{-\lambda_j y_j^2/2\varepsilon} \,\mathrm{d}y_j \biggl[1 + \mathcal{O}\biggl(\frac{[\delta + \delta_1 + \delta_2]^{2r+1}}{\varepsilon}\biggr)\biggr] . \tag{4.16}$$

Using the fact that the Gaussian integrals over y_j, $j = 2, \dots, d$, are bounded above by $\sqrt{2\pi\varepsilon/\lambda_j}$, the desired bound (4.4) follows. □

Remark 4.2. Using the conditions (4.2) in order to bound the integrals over y_1 and y_2, one obtains as a rough a priori bound

$$\operatorname{cap}_A(B) \leqslant const \frac{\delta_2}{\delta_1} \varepsilon^{-(c+1/2)d} . \tag{4.17}$$

In applications we will of course obtain much sharper bounds by using explicit expressions for $u_1(y_1)$ and $u_2(y_2)$, but the above rough bound will be sufficient in order to obtain a lower bound on the capacity, valid without further knowledge of the functions u_1 and u_2.

4.2 Lower bound

Before we proceed to deriving a lower bound on the capacity, we need a crude bound on the equilibrium potential $h_{A,B}$. We obtain such a bound by adapting similar results from [BEGK04, Section 4] to the present situation.

Lemma 4.3. *Let A and B be disjoint sets, and let $x \in (A \cup B)^c$ be such that the ball $\mathcal{B}(x, \varepsilon)$ does not intersect $A \cup B$. Then there exists a constant C such that*

$$h_{A,B}(x) \leqslant C\varepsilon^{-d} \operatorname{cap}_{\mathcal{B}_\varepsilon(x)}(A) \,\mathrm{e}^{\overline{V}(\{x\},B)/\varepsilon} . \tag{4.18}$$

PROOF: [BEGK04, Proposition 4.3] provides the upper bound

$$h_{A,B}(x) \leqslant C \frac{\operatorname{cap}_{\mathcal{B}_\varepsilon(x)}(A)}{\operatorname{cap}_{\mathcal{B}_\varepsilon(x)}(B)} , \tag{4.19}$$

so that it suffices to obtain a lower bound for the denominator. This is done as in [BEGK04, Proposition 4.7] with $\rho = \varepsilon$, cf. in particular Equation (4.26) in that work, which provides a lower bound for the capacity in terms of an integral of $\mathrm{e}^{V/\varepsilon}$ over a critical path from x to B. Evaluating the integral by the Laplace method, one gets $\mathrm{e}^{\overline{V}(\{x\},B)/\varepsilon}$ as leading term, with a multiplicative correction. The only difference is that while Bovier *et al* assume quadratic saddles, which yields a correction of order $\sqrt{\varepsilon}$, here we do not assume anything on the saddles, so that in the worst case the prefactor is constant. This yields the bound (4.18). □

The capacity $\operatorname{cap}_{\mathcal{B}_\varepsilon(x)}(A)$ behaves roughly like $\mathrm{e}^{-\overline{V}(\{x\},A)/\varepsilon}$, so that the bound (4.18) is useful whenever $\overline{V}(\{x\},A) \gg \overline{V}(\{x\},B)$. This is the case, in particular, when A and B belong to different path-connected components of the open valley of a saddle z, and x belongs to the same component as B. If, by contrast, x belongs to the same component as A, the symmetry $h_{A,B}(x) = 1 - h_{B,A}(x)$ yields a lower bound for the equilibrium potential which is close to 1.

We now consider the same situation as in Section 4.1. Let $\delta_1(\varepsilon)$, $\delta_2(\varepsilon)$ and c be the constants introduced in Proposition 4.1.

Proposition 4.4 (The lower bound)**.** *Assume that $\delta_2(\varepsilon)/\delta_1(\varepsilon) \leqslant \varepsilon^{-q}$ for some $q \in \mathbb{R}$, and let $K = \max\{q + \frac{1}{2} + (c + \frac{3}{2})d, 1\}$. Assume there exist strictly positive numbers $\hat{\delta}_1 = \hat{\delta}_1(\varepsilon)$ and $\hat{\delta}_2 = \hat{\delta}_2(\varepsilon)$ such that*

$$\begin{aligned} u_1(\pm\hat{\delta}_1) &\geqslant 4K\varepsilon|\log\varepsilon| , \\ u_2(y_2) &\leqslant K\varepsilon|\log\varepsilon| \qquad\qquad \text{whenever } |y_2| \leqslant \hat{\delta}_2 , \end{aligned}$$

and such that

$$\big[\hat{\delta}_1(\varepsilon) + \hat{\delta}_2(\varepsilon)\big]^{2r+1} = \mathcal{O}(\varepsilon|\log\varepsilon|) . \tag{4.20}$$

Then

$$\operatorname{cap}_A(B) \geqslant \varepsilon \frac{\displaystyle\int_{-\hat{\delta}_2}^{\hat{\delta}_2} \mathrm{e}^{-u_2(y_2)/\varepsilon} \, \mathrm{d}y_2}{\displaystyle\int_{-\hat{\delta}_1}^{\hat{\delta}_1} \mathrm{e}^{-u_1(y_1)/\varepsilon} \, \mathrm{d}y_1} \prod_{j=3}^{d} \sqrt{\frac{2\pi\varepsilon}{\lambda_j}} \big[1 - R_3(\varepsilon)\big] , \tag{4.21}$$

where the remainder $R_3(\varepsilon)$ satisfies

$$R_3(\varepsilon) \leqslant C\big[\varepsilon^{r-1/2}|\log\varepsilon|^{r+1/2} + \varepsilon^{-1}(\hat{\delta}_1^{2r+1} + \hat{\delta}_2^{2r+1}) + \hat{\delta}_1 + \hat{\delta}_2 + \sqrt{\varepsilon}\big] \tag{4.22}$$

for some constant $C > 0$.

PROOF: As in the proof of Proposition 4.1, we start by locally carrying out the normal form transformation in the integral defining the Dirichlet form. Next we define a slightly different neighbourhood of the saddle,

$$\widehat{C}_\varepsilon = \prod_{j=1}^{d} [-\hat{\delta}_j, \hat{\delta}_j] = [-\hat{\delta}_1, \hat{\delta}_1] \times \widehat{C}_\varepsilon^\perp , \tag{4.23}$$

where we now choose

$$\hat{\delta}_j = \frac{\delta}{\sqrt{(d-2)\lambda_j}} , \quad j = 3, \dots, d , \tag{4.24}$$

with $\delta = \sqrt{K\varepsilon|\log\varepsilon|}$. The reason for this choice is that we want the potential to be smaller than $-\delta^2$ on the "sides" $\{\pm\hat{\delta}_1\} \times \widehat{C}_\varepsilon^\perp$ of the box. Indeed, we have

$$\begin{aligned} \frac{V(\pm\hat{\delta}_1, y_\perp)}{\varepsilon} &\leqslant -4K|\log\varepsilon| + K|\log\varepsilon| + (d-2)\frac{\delta^2}{2\varepsilon(d-2)} + \mathcal{O}\bigl(\varepsilon^{-1}[\delta + \hat{\delta}_1 + \hat{\delta}_2]^{2r+1}\bigr) \\ &\leqslant -K|\log\varepsilon| \end{aligned} \tag{4.25}$$

for sufficiently small ε. As a consequence, if $h^\star = h_{A,B}$ denotes the equilibrium potential, Lemma 4.3 and (4.17) yield

$$h^\star(\hat{\delta}_1, y_\perp) = \mathcal{O}\bigl(\varepsilon^{-d}\varepsilon^{-q}\varepsilon^{-(c+1/2)d}\,\mathrm{e}^{V(\hat{\delta}_1,y_\perp)/\varepsilon}\bigr) = \mathcal{O}\bigl(\varepsilon^{-q-(c+3/2)d+K}\bigr) = \mathcal{O}\bigl(\varepsilon^{1/2}\bigr) \tag{4.26}$$

while

$$h^\star(-\hat{\delta}_1, y_\perp) = 1 - \mathcal{O}\bigl(\varepsilon^{1/2}\bigr) . \tag{4.27}$$

We can now proceed to deriving the lower bound. Observe that

$$\operatorname{cap}_A(B) = \Phi_{(A\cup B)^c}(h^\star) \geqslant \Phi_{\widehat{C}_\varepsilon}(h^\star) . \tag{4.28}$$

Now we can write, for any $h \in \mathcal{H}_{A,B}$,

$$\begin{aligned} \Phi_{\widehat{C}_\varepsilon}(h) &\geqslant \varepsilon \int_{\widehat{C}_\varepsilon} \mathrm{e}^{-V(y)/\varepsilon} \biggl(\frac{\partial h}{\partial y_1}\biggr)^2 \,\mathrm{d}y \\ &= \varepsilon \int_{\widehat{C}_\varepsilon^\perp} \int_{-\hat{\delta}_1}^{\hat{\delta}_1} \mathrm{e}^{-V(y)/\varepsilon} \biggl(\frac{\partial h(y_1, y_\perp)}{\partial y_1}\biggr)^2 \,\mathrm{d}y_1\,\mathrm{d}y_\perp , \end{aligned}$$

and thus

$$\Phi_{\widehat{C}_\varepsilon}(h^\star) \geqslant \varepsilon \int_{\widehat{C}_\varepsilon^\perp} \biggl[\inf_{f\colon f(\pm\hat{\delta}_1) = h^\star(\pm\hat{\delta}_1, y_\perp)} \int_{-\hat{\delta}_1}^{\hat{\delta}_1} \mathrm{e}^{-V(y)/\varepsilon} f'(y_1)^2 \,\mathrm{d}y_1 \biggr] \mathrm{d}y_\perp . \tag{4.29}$$

The Euler–Lagrange equation for the variational problem is

$$\varepsilon f''(y_1) - \frac{\partial V}{\partial y_1}(y_1, y_\perp) f'(y_1) = 0 \tag{4.30}$$

with boundary conditions $h^\star(-\hat{\delta}_1, y_\perp)$ in $-\hat{\delta}_1$ and $h^\star(\hat{\delta}_1, y_\perp)$ in $\hat{\delta}_1$, and has the solution

$$f(y_1) = h^\star(\hat{\delta}_1, y_\perp) - \bigl[h^\star(\hat{\delta}_1, y_\perp) - h^\star(-\hat{\delta}_1, y_\perp)\bigr] \frac{\displaystyle\int_{y_1}^{\hat{\delta}_1} \mathrm{e}^{V(t,y_\perp)/\varepsilon}\,\mathrm{d}t}{\displaystyle\int_{-\hat{\delta}_1}^{\hat{\delta}_1} \mathrm{e}^{V(t,y_\perp)/\varepsilon}\,\mathrm{d}t} . \tag{4.31}$$

As a consequence,

$$f'(y_1) = \bigl[h^\star(\hat{\delta}_1, y_\perp) - h^\star(-\hat{\delta}_1, y_\perp)\bigr] \frac{\mathrm{e}^{V(y_1,y_\perp)/\varepsilon}}{\displaystyle\int_{-\hat{\delta}_1}^{\hat{\delta}_1} \mathrm{e}^{V(t,y_\perp)/\varepsilon}\,\mathrm{d}t} , \tag{4.32}$$

so that substitution in (4.29) yields

$$\Phi_{\widehat{C}_\varepsilon}(h^\star) \geqslant \varepsilon \int_{\widehat{C}_\varepsilon^\perp} \frac{\bigl[h^\star(\hat\delta_1, y_\perp) - h^\star(-\hat\delta_1, y_\perp)\bigr]^2}{\displaystyle\int_{-\hat\delta_1}^{\hat\delta_1} \mathrm{e}^{V(t,y_\perp)/\varepsilon} \,\mathrm{d}t} \,\mathrm{d}y_\perp \;. \tag{4.33}$$

The bounds (4.26) and (4.27) on $h^\star$ show that the numerator is of the form $1 - \mathcal{O}(\varepsilon^{1/2})$. It now suffices to use the normal form (4.1) of the potential, and to perform the integrals over $y_3, \dots y_d$. □

4.3 Proofs of the main results

PROOF OF THEOREM 3.1. For the upper bound, it suffices to apply Proposition 4.1 in the case $u_1(y_1) = C_4 y_1^4$ and $u_2(y_2) = \lambda_2 y_2^2/2$. The conditions for the upper bound are fulfilled for $\delta_1 = (d\varepsilon|\log\varepsilon|/C_4)^{1/4}$, $\delta_2 = 2(d\varepsilon|\log\varepsilon|/\lambda_2)^{1/2}$ and $c = 0$. This yields error terms $R_1(\varepsilon) = \mathcal{O}(\varepsilon^{1/4}|\log\varepsilon|^{1/4})$ and $R_2(\varepsilon) = \mathcal{O}(\varepsilon^{d/2+3/5})$. The integrals over y_1 and y_2 can be computed explicitly (extending their bounds to $\pm\infty$ only produces a negligible error). A matching lower bound is obtained in a completely analogous way, using Proposition 4.4. □

PROOF OF THEOREM 3.4. The proof is essentially the same as the previous one, only with the rôles of δ_1 and δ_2 interchanged. □

PROOF OF THEOREM 3.7. We decompose the proof into several steps.

Proposition 4.5. *Under the assumptions of Theorem 3.7, and for $\lambda_2 > 0$,*

$$\operatorname{cap}_A(B) = \frac{I_{a,\varepsilon}}{(2C_4)^{1/4}} \sqrt{\frac{(2\pi)^{d-3}|\lambda_1|}{\lambda_3 \dots \lambda_d}} \varepsilon^{d/2-1/2} \,\mathrm{e}^{-V(z)/\varepsilon} \bigl[1 + R_+(\varepsilon)\bigr] \;, \tag{4.34}$$

where $R_+(\varepsilon)$ is defined in (3.27), *$I_{a,\varepsilon}$ is the integral*

$$I_{a,\varepsilon} = \int_{-\infty}^{\infty} \mathrm{e}^{-(x^4 + a x^2)/2\varepsilon} \,\mathrm{d}x \;, \tag{4.35}$$

and $a = \lambda_2/\sqrt{2C_4}$.

PROOF: It suffices to apply Propositions 4.1 and 4.4, taking some care in the choice of the δ_i. The conditions yield $\delta_1 = (2d\varepsilon|\log\varepsilon|/|\lambda_1|)^{1/2}$ and

$$\delta_2^2 = \frac{-\lambda_2 + \sqrt{\lambda_2^2 + 32 d C_4 \varepsilon|\log\varepsilon|}}{4C_4} \;. \tag{4.36}$$

For $\lambda_2 > (\varepsilon|\log\varepsilon|)^{1/2}$, this implies that δ_2 has order $(\varepsilon|\log\varepsilon|/\lambda_2)^{1/2}$, while for $0 < \lambda_2 < (\varepsilon|\log\varepsilon|)^{1/2}$, it yields δ_2 of order $(\varepsilon|\log\varepsilon|)^{1/4}$. The expressions of $\hat\delta_1$ and $\hat\delta_2$ are similar. This yields the announced error terms. The integral over y_1 is carried out explicitly, while the integral over y_2 equals $I_{a,\varepsilon}/(2C_4)^{1/4}$, up to a negligible error term. □

Proposition 4.6. *Under the assumptions of Theorem 3.7, and for* $\lambda_2 < 0$,

$$\operatorname{cap}_A(B) = \frac{J_{b,\varepsilon}}{(2C_4)^{1/4}} \sqrt{\frac{(2\pi)^{d-3}|\mu_1|}{\mu_3 \dots \mu_d}} \varepsilon^{d/2-1/2} \,\mathrm{e}^{-V(z_\pm)/\varepsilon} \big[1 + R_-(\varepsilon)\big] \;, \tag{4.37}$$

where $R_-(\varepsilon)$ *is defined in* (3.27), $J_{b,\varepsilon}$ *is the integral*

$$J_{b,\varepsilon} = \int_{-\infty}^{\infty} \mathrm{e}^{-(x^2-b/4)^2/2\varepsilon} \,\mathrm{d}x \;, \tag{4.38}$$

and $b = \mu_2/\sqrt{2C_4}$.

Proof: First note that for small negative λ_2,

$$u_2(y_2) = C_4 \biggl(y_2^2 - \frac{\mu_2}{8C_4}\biggr)^2 - \frac{\mu_2^2}{64C_4} + \mathcal{O}(|\lambda_2|^{5/2}) + \mathcal{O}(|\lambda_2|^{3/2} y_2^2) \;, \tag{4.39}$$

where the constant term corresponds to $V(z_\pm) - V(z)$. The situation is more difficult than before, because $u_2(y_2)$ is not increasing on $\mathbb{R}_+$. When applying Proposition 4.1, we distinguish two regimes.

- For $\mu_2 < (\varepsilon|\log\varepsilon|)^{1/2}$, it is sufficient to choose δ_2 of order $(\varepsilon|\log\varepsilon|)^{1/4}$.
- For $\mu_2 \geqslant (\varepsilon|\log\varepsilon|)^{1/2}$, we cannot apply Proposition 4.1 as is, but first split the integral over y_2 into the integrals over $\mathbb{R}_+$ and over $\mathbb{R}_-$. Each integral is in fact dominated by the integral over an interval of order $(\varepsilon|\log\varepsilon|/\mu_2)^{1/2}$ around the minimum $y_2 = \pm(\mu_2/8C_4)^{1/2}$, so that one can choose δ_2 of that order.

We make a similar distinction between regimes when choosing $\hat\delta_2$ in order to apply Proposition 4.4. This yields the announced error terms, and the integrals are treated as before. □

In order to complete the proof of Theorem 3.7, it remains to examine the integrals $I_{a,\varepsilon}$ and $J_{b,\varepsilon}$. First note that

$$I_{a,\varepsilon} = \sqrt{\frac{2\pi\varepsilon^{1/2}}{1+\alpha}} \Psi_+(\alpha) \;, \tag{4.40}$$

where $\alpha = a/\sqrt{\varepsilon}$ and

$$\Psi_+(\alpha) = \sqrt{\frac{1+\alpha}{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-(y^4+\alpha y^2)/2} \,\mathrm{d}y \;. \tag{4.41}$$

The change of variables $y = z/\sqrt{1+\alpha}$ yields

$$\Psi_+(\alpha) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\biggl\{-\frac12 \biggl[\frac{z^4}{(1+\alpha)^2} + \frac{\alpha z^2}{1+\alpha}\biggr]\biggr\} \,\mathrm{d}z \;, \tag{4.42}$$

which allows to show that Ψ_+ is bounded above and below by positive constants, and to compute the limits as $\alpha \to 0$ and $\alpha \to \infty$. The expressions in terms of Bessel functions are obtained by observing that

$$f(\delta) := \int_{-\infty}^{\infty} \exp\biggl\{-12 \biggl[y^4 + 2\delta y^2 + \frac{\delta^2}{2}\biggr]\biggr\} \,\mathrm{d}y = \sqrt{\frac{\delta}{2}} K_{1/4}\biggl(\frac{\delta^2}{4}\biggr) \;, \tag{4.43}$$

because it satisfies the equation $f''(\delta) = (\delta^2/4) f(\delta)$. The other integral is treated in a similar way. □

A Normal forms

Proof of Proposition 2.8. Let us denote by $\mathcal{G}_k(n,m)$ the vector space of functions $g\colon \mathbb{R}^n \to \mathbb{R}^m$ which are homogeneous of degree k (i.e., $g(tx) = t^k g(x)\ \forall x$). We write the Taylor series of V in the form

$$V(x) = V_2(x) + V_3(x) + V_4(x) + \mathcal{O}(\|x\|_2^4)\ , \tag{A.1}$$

where $V_k \in \mathcal{G}_k(d,1)$ for $k = 2,3,4$. We first look for a function $g \in \mathcal{G}_2(d,d)$ such that $V \circ [\mathrm{id} + g_2]$ contains as few terms of order 3 as possible. The Taylors series of $V \circ [\mathrm{id} + g_2]$ can be written

$$\begin{aligned} &V(x + g_2(x)) \\ &\quad = V_2(x) + \underbrace{\nabla V_2(x)\cdot g_2(x) + V_3(x)}_{\text{order 3}} + \underbrace{V_2(g_2(x)) + \nabla V_3(x)\cdot g_2(x) + V_4(x)}_{\text{order 4}} + \mathcal{O}(\|x\|_2^4)\ . \end{aligned} \tag{A.2}$$

Now consider the so-called adjoint map $T\colon \mathcal{G}_2(d,d) \to \mathcal{G}_3(d,1)$, $g_2 \mapsto \nabla V_2(\cdot)\cdot g_2$, seen as a linear map between vector spaces. All terms of $V_3(x)$ in the image of T can be eliminated by a suitable choice of g_2. Let e_l denote the lth vector in the canonical basis of $\mathbb{R}^d$. We see that

$$T(x_j x_k e_l) = \lambda_l x_j x_k x_l \neq 0 \qquad \text{for } l = 2,\dots,d\ . \tag{A.3}$$

Thus all monomials except x_1^3 are in the image of T. Since T involves multiplication by x_2 or x_3 or $\dots$ or x_d, however, x_1^3 is not in the image of T. Hence this term is resonant. We can thus choose g_2 in such a way that

$$V(x + g_2(x)) = V_2(x) + \underbrace{V_{111}x_1^3}_{\text{order 3}} + \underbrace{V_2(g_2(x)) + \nabla V_3(x)\cdot g_2(x) + V_4(x)}_{\text{order 4}} + \mathcal{O}(\|x\|_2^4)\ . \tag{A.4}$$

Now a completely analogous argument shows that we can construct a function $g_3 \in \mathcal{G}_3(d,d)$ such that $V \circ [\mathrm{id} + g_3] \circ [\mathrm{id} + g_2]$ has some constant times x_1^4 as the only term of order 4. It remains to determine this constant. From (A.4) we deduce that it has the expression

$$C_4 = \frac{1}{2}\sum_{j=2}^{d} \lambda_j (g_{11}^j)^2 + \sum_{j=1}^{d} V_{11j} g_{11}^j + V_{1111}\ , \tag{A.5}$$

where g_{11}^j denotes the coefficient of $x_1^2 e_j$ in g_2. The expression of T shows that necessarily $g_{11}^j = -V_{11j}/\lambda_j$ for $j = 2,\dots,d$, while we may choose $g_{11}^1 = 0$. This yields (2.14). □

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