Reactive trajectories and the transition path process

Jianfeng Lu · James Nolen

Abstract We study the trajectories of a solution X_t to an Itô stochastic differential equation in $\mathbb{R}^d$, as the process passes between two disjoint open sets, A and B. These segments of the trajectory are called transition paths or reactive trajectories, and they are of interest in the study of chemical reactions and thermally activated processes. In that context, the sets A and B represent reactant and product states. Our main results describe the probability law of these transition paths in terms of a transition path process Y_t, which is a strong solution to an auxiliary SDE having a singular drift term. We also show that statistics of the transition path process may be recovered by empirical sampling of the original process X_t. As an application of these ideas, we prove various representation formulas for statistics of the transition paths. We also identify the density and current of transition paths. Our results fit into the framework of the transition path theory by Weinan and Vanden-Eijnden.

Keywords Transition path process · Reactive trajectory · Stochastic differential equations

Mathematics Subject Classification 60H10 · 60H30

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1 Introduction

In this article we study solutions $X_t \in \mathbb{R}^d$ of the Itô stochastic differential equation

$$\mathrm{d}X_t = b(X_t)\,\mathrm{d}t + \sqrt{2}\,\sigma(X_t)\,\mathrm{d}W_t, \tag{1.1}$$

where $(W_t, \mathcal{F}_t^W)$ is a standard Brownian motion in $\mathbb{R}^d$, defined on a probability space $(\Omega, \mathcal{F}, \mathbb{P})$. This diffusion process in $\mathbb{R}^d$ has generator

$$Lu = \mathrm{tr}(a\nabla^2 u) + b \cdot \nabla u,$$

where $a := \sigma\sigma^{\mathrm{T}}$ is a symmetric matrix. We suppose that $\sigma(x)$ is smooth and that $a(x)$ is uniformly positive definite and bounded:

$$\lambda|\xi|^2 \le \langle \xi, a(x)\xi \rangle \le \Lambda|\xi|^2, \quad \forall\, \xi \in \mathbb{R}^d, \quad \forall\, x \in \mathbb{R}^d \tag{1.2}$$

holds for some $\Lambda > \lambda > 0$. Although the vector field b may not be bounded, we suppose that b is smooth and satisfies conditions that guarantee the ergodicity of the Markov process X_t and the existence of a unique invariant probability distribution $\rho(x) > 0$ satisfying the adjoint equation

$$L^*\rho = (a_{ij}(x)\rho(x))_{x_i x_j} - \nabla \cdot (b(x)\rho(x)) = 0. \tag{1.3}$$

We also assume that for some $\alpha > 1$,

$$\sup_{|x|<R} \mathbb{E}[\,\tau_1^\alpha \mid X_0 = x\,] < +\infty \tag{1.4}$$

for all $R > 0$, where τ_1 is the first hitting time of X_t to the unit ball $\{z \in \mathbb{R}^d \mid |z| \le 1\}$. For example, it follows from Theorems 2 and 3 of [34] that these assumptions will hold if

$$\limsup_{m \to +\infty} \sup_{|x|=m} x \cdot b(x) < -r$$

for some $r > 1 + (d/2)$.

Suppose that $A, B \subset \mathbb{R}^d$ are two bounded open sets with smooth boundary and such that $\overline{A}$ and $\overline{B}$ are disjoint. Because the process is ergodic, X_t will visit both A and B infinitely often. Inspired by the transition path theory developed by Weinan E and Vanden-Eijnden [15,24] (see also the review article [16]), our main interest is in those segments of the trajectory $t \mapsto X_t$ which pass from A to B. These transition paths and are defined precisely as follows. First, for $k \ge 0$, define the hitting times $\tau_{A,k}^+$ and $\tau_{B,k}^+$ inductively by

$$\tau_{A,0}^+ = \inf\left\{t \ge 0 \mid X_t \in \overline{A}\right\},$$
$$\tau_{B,0}^+ = \inf\left\{t > \tau_{A,0}^+ \mid X_t \in \overline{B}\right\},$$
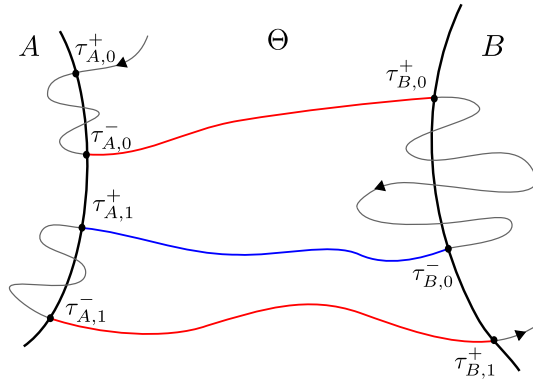
Fig. 1 Illustration of a trajectory with entrance and exit times. The transition path from A to B is marked in *red* (color figure online)

and for $k \geq 0$,

$$\tau_{A,k+1}^+ = \inf\left\{t > \tau_{B,k}^+ \mid X_t \in \overline{A}\right\},$$

$$\tau_{B,k+1}^+ = \inf\left\{t > \tau_{A,k+1}^+ \mid X_t \in \overline{B}\right\}.$$

We will call these the **entrance times**. Then define the **exit times**

$$\tau_{A,k}^- = \sup\left\{t < \tau_{B,k}^+ \mid X_t \in \overline{A}\right\},$$

$$\tau_{B,k}^- = \sup\left\{t < \tau_{A,k+1}^+ \mid X_t \in \overline{B}\right\}.$$

These times are all finite with probability one, and $\tau_{A,k}^+ \leq \tau_{A,k}^- < \tau_{B,k}^+ \leq \tau_{B,k}^- < \tau_{A,k+1}^+$ for all $k \geq 0$ (see Fig. 1). If $t \in [\tau_{A,k}^-, \tau_{B,k}^+]$ for some k, we say that the path X_t is $A \to B$ **reactive**. Let $\Theta = (A \cup B)^c$, and hence $\partial \Theta = \partial A \cup \partial B$. For $k \in \mathbb{N}$, the continuous process $Y^k : [0, \infty) \to \overline{\Theta}$ defined by

$$Y_t^k = X_{(t+\tau_{A,k}^-)\wedge\tau_{B,k}^+} \tag{1.5}$$

is the kth $A \to B$ **reactive trajectory** or **transition path**. Observe that $Y_0^k = X_{\tau_{A,k}^-} \in \partial A$, that $Y_t^k = X_{\tau_{B,k}^+} \in \partial B$ for all $t \geq \tau_{B,k}^+ - \tau_{A,k}^-$, and that $Y_t^k \in \Theta$ for all $t \in (0, \tau_{B,k}^+ - \tau_{A,k}^-)$. Unlike the entrance times, the exit times $\tau_{A,k}^-$ and $\tau_{B,k}^-$ are not stopping times with respect to the natural filtration. So, one cannot apply the strong Markov property to X_t at times $\tau_{A,k}^-$ and $\tau_{B,k}^-$. Indeed, the law of the process Y_t^k is very different from that of the process X_t starting at a point in ∂A.

Our main results describe the probability law of these transition paths in terms of a **transition path process**, which is a strong solution to an auxiliary stochastic differential equation. In particular, empirical samples of the reactive portions of X_t may be regarded as sampling from the transition path process. The motivation comes from

the study of chemical reactions and thermally activated processes where understanding these reactive trajectories are crucial [6,12]. In these applications, the domains A and B are usually chosen as regions in configurational space corresponding to reactant and product states. Mathematically, our results fit into the framework of the transition path theory [15,16,24].

Having identified the transition path process, we can compute statistics of the transition paths by sampling directly from the transition path SDE, rather than using acceptance/rejection methods or very long-time integration on the original SDE. Our theoretical results might be used to analyze numerical methods of sampling reactive trajectories.

We will now describe our main results and their relation to other works. Proofs are deferred to later sections.

1.1 The transition path process

Our definition of the transition path process is motivated by the Doob h-transform as follows. Let τ_A and τ_B denote the first hitting time of X_t to the sets $\overline{A}$ and $\overline{B}$, respectively:

$$\begin{aligned} \tau_A &= \inf\left\{ t \geq 0 \mid X_t \in \overline{A} \right\}, \\ \tau_B &= \inf\left\{ t \geq 0 \mid X_t \in \overline{B} \right\}. \end{aligned} \tag{1.6}$$

Let $q(x) \geq 0$ be the **forward committor function**:

$$q(x) = \mathbb{P}(\tau_A > \tau_B \mid X_0 = x), \tag{1.7}$$

which satisfies $Lq(x) = 0$ for $x \in \Theta = (A \,\overline{\cup}\, B)^c$ and

$$q(x) = \begin{cases} 0, & x \in \overline{A}, \\ 1, & x \in \overline{B}. \end{cases} \tag{1.8}$$

By the maximum principle, $q(x) > 0$ for all $x \in \Theta$. By the Hopf lemma we also have

$$\sup_{x \in \partial A} \widehat{n}(x) \cdot \nabla q(x) < 0, \qquad \inf_{x \in \partial B} \widehat{n}(x) \cdot \nabla q(x) > 0, \tag{1.9}$$

where $\widehat{n}(x)$ will denote the unit normal exterior to Θ (pointing into A and B). For $x \in \Theta$, consider the stopped process $X_{t \wedge \tau_A \wedge \tau_B}$ with $X_0 = x$, and let $\mathcal{P}_x$ denote the corresponding measure on $\mathcal{X} = C([0, \infty), \Theta)$:

$$\mathcal{P}_x(U) = \mathbb{P}(X \in U \mid X_0 = x), \quad \forall\, U \in \mathcal{B}$$

where $\mathcal{B}$ is the Borel σ-algebra on $\mathcal{X}$. If Λ_{AB} denotes the event that $\tau_A > \tau_B$, the measure $\mathcal{Q}_x^q$ on $(\mathcal{X}, \mathcal{B})$ defined by

$$\frac{d\mathcal{Q}_x^q}{d\mathcal{P}_x} = \frac{\mathbb{I}_{\Lambda_{AB}}}{\mathcal{P}_x(\Lambda_{AB})} = \frac{\mathbb{I}_{\Lambda_{AB}}}{q(x)}$$

is absolutely continuous with respect to $\mathcal{P}_x$, if $x \in \Theta$. By the Doob h-transform (see e.g. [28, Theorem 7.2.2]), we know that $\mathcal{Q}_x^q$ defines a diffusion process Y_t on $C([0, \infty), \overline{\Theta})$ with generator:

$$L^q f = \frac{1}{q} L(qf) = \text{tr}(a\nabla^2 f) + (b \cdot \nabla f) + \frac{2a\nabla q}{q} \cdot \nabla f = Lf + \frac{2a\nabla q}{q} \cdot \nabla f. \quad (1.10)$$

So, the effect of conditioning on the event $\tau_B < \tau_A$ is to introduce an additional drift term. For $x \in \Theta$, the transition probability for Y_t is

$$p^q(t, x, dy) = \frac{1}{q(x)} p(t, x, dy) q(y) \quad (1.11)$$

where $p(t, x, dy)$ is the transition probability for X_t killed at ∂B [28, Theorem 4.1.1].

This observation suggests that the $A \to B$ reactive trajectories should have the same law as a solution to the SDE

$$dY_t = \left(b(Y_t) + \frac{2a(Y_t)\nabla q(Y_t)}{q(Y_t)} \right) dt + \sqrt{2}\,\sigma(Y_t)\,d\widehat{W}_t, \quad (1.12)$$

originating at a point $Y_0 = y_0 \in \partial A$ and terminating at a point in ∂B. While the SDE (1.12) admits strong solutions for $y_0 \in \Theta$ since $q(x) > 0$ in Θ, the drift term becomes singular at the boundary of A, where q vanishes. Our first result is the following theorem which shows that there is still a unique strong solution to this SDE even for initial condition lying in ∂A. For convenience, let us define the vector field

$$K(y) = \left(b(y) + \frac{2a(y)\nabla q(y)}{q(y)} \right). \quad (1.13)$$

Theorem 1.1 *Let $(\widehat{W}, \mathcal{F}_t^{\widehat{W}})$ be a standard Brownian motion in $\mathbb{R}^d$, defined on a probability space $(\widehat{\Omega}, \widehat{\mathcal{F}}, \mathbb{Q})$. Let $\xi : \widehat{\Omega} \to \overline{\Theta}$ be a random variable defined on the same probability space and independent of $\widehat{W}$. There is a unique, continuous process $Y_t : [0, \infty) \to \overline{\Theta}$ which is adapted to the augmented filtration $\widehat{\mathcal{F}}_t$ and satisfying the following, $\mathbb{Q}$-almost surely:*

$$Y_t = \xi + \int_0^{t \wedge \tau_B} K(Y_s)\,ds + \int_0^{t \wedge \tau_B} \sqrt{2}\,\sigma(Y_s)\,d\widehat{W}_s, \quad t \geq 0 \quad (1.14)$$

where

$$\tau_B = \inf\{t > 0 \mid Y_t \in \overline{B}\}.$$

Moreover, $Y_t \notin \overline{A}$ for all $t > 0$.

The augmented filtration is defined in the usual way, $\widehat{\mathcal{F}}_t$ being the σ-algebra generated by $\mathcal{F}_t^{\widehat{W}}$, Y_0, and the appropriate collection of null sets so that $\widehat{\mathcal{F}}_t$ is both left- and right- continuous. We will use $\widehat{\mathbb{E}}$ to denote expectation with respect to the probability measure $\mathbb{Q}$.

Observe that if $d = 1$, $\sigma = 1/\sqrt{2}$ is constant, and $b \equiv 0$, then $q(x)$ is a linear function, and (1.12) corresponds to a Bessel process of dimension 3. For example, if $A = (-\infty, 0)$, $B = (1, \infty)$, we have

$$\mathrm{d}Y_t = \frac{1}{Y_t}\,\mathrm{d}t + \mathrm{d}\widehat{W}_t,$$

and the function $Z_t = (Y_t)^2$ satisfies the degenerate diffusion equation

$$\mathrm{d}Z_t = 3\,\mathrm{d}t + 2\sqrt{Z_t}\,\mathrm{d}\widehat{W}_t. \tag{1.15}$$

In this simple case, existence and uniqueness of a strong solution starting at $Y_0 = 0$ can be shown using arguments involving Brownian local time (see [23,30]). However, those arguments are not applicable to the more general setting we consider here. The work most closely related to Theorem 1.1 in a higher dimensional setting may be that of DeBlaissie [14] who proved pathwise uniqueness for certain SDEs having diffusion coefficients that degenerate like $\sqrt{d(Z_t)}$ where $d(z)$ is the distance to the domain boundary (as in (1.15)). In an earlier work, Athreya et al. [1] proved uniqueness for the martingale problem associated with a similarly degenerate diffusion in a positive orthant in $\mathbb{R}^d$. Nevertheless, those analyses do not apply to the case (1.12) considered here.

The next theorem shows that the law of the reactive trajectories is that of the process Y_t with appropriate initial condition. For this reason, we will call the process Y_t the **transition path process**.

Theorem 1.2 *Let X_t satisfy the SDE (1.1). Let Y^k denote the kth $A \to B$ reactive trajectory defined by (1.5). Let Y be defined as in Theorem 1.1. Then for any bounded and continuous functional $F : C([0, \infty)) \to \mathbb{R}$, we have*

$$\mathbb{E}[F(Y^k)] = \widehat{\mathbb{E}}\left[F(Y) \mid Y_0 \sim X_{\tau_{A,k}^-}\right].$$

The processes X_t and Y_t^k may be defined on a probability space that is different from the one on which Y_t is defined. The notation $Y_0 \sim X_{\tau_{A,k}^-}$ used in Theorem 1.2 means that Y_0 has the same law as $X_{\tau_{A,k}^-}$, meaning $\mathbb{Q}(Y_0 \in U) = \mathbb{P}(X_{\tau_{A,k}^-} \in U)$ for any Borel set $U \subset \mathbb{R}^d$.

1.2 Reactive exit and entrance distributions

The distribution of the random points $X_{\tau_{A,k}^-}$ will depend in the initial condition X_0. From the point of view of sampling the transition paths, however, there is a very

natural distribution to consider for Y_0, which is related to the "equilibrium measure" in the potential theory for diffusion processes [7,8,32]. To motivate this distribution formally, let $h > 0$ and consider the regularized hitting times

$$\tau_{A,h} = \inf \left\{ t \geq h \mid X_t \in \overline{A} \right\} \tag{1.16}$$

$$\tau_{B,h} = \inf \left\{ t \geq h \mid X_t \in \overline{B} \right\}, \tag{1.17}$$

where X_t satisfies (1.1). Then define

$$q_h(x) = \mathbb{P}(\tau_{A,h} > \tau_{B,h} \mid X_0 = x).$$

This is the probability that at some time $s \in [0, h]$, the path X_t starting from $x \in \partial A$ becomes a transition path, not returning to $\overline{A}$ before hitting $\overline{B}$. With this in mind, the quantity

$$\eta_{A,h}(x) = h^{-1}\rho(x)\mathbb{P}(\tau_{A,h} > \tau_{B,h} \mid X_0 = x) = h^{-1}\rho(x)q_h(x),$$

may be interpreted as a rate at which transition paths exit A, when the system is in equilibrium. Therefore, a natural choice for an initial distribution for $Y_0 \in \partial A$ is:

$$\eta_A(x) = \lim_{h \to 0} \eta_{A,h}.$$

By the Markov property, we have

$$q_h(x) = \int_{\mathbb{R}^d} \mathbb{P}(\tau_A > \tau_B \mid X_0 = y)\rho(h, x, y)\, \mathrm{d}y = \mathbb{E}[q(X_h) \mid X_0 = x] \tag{1.18}$$

where $\rho(t, x, \cdot)$ is the density for X_t, given $X_0 = x$. Therefore, for any $x \in \partial A$ we have

$$\lim_{h \to 0} h^{-1}q_h(x) = \lim_{h \to 0} h^{-1}\mathbb{E}[q(X_h) - q(X_0) \mid X_0 = x] = Lq(x),$$

in the sense of distributions, although q is not C^2 on $\partial\Theta = \partial A \cup \partial B$. Hence $\eta_{A,h}(x) \to \eta_A(x) = \rho(x)Lq(x)$ for $x \in \partial A$. The distribution Lq is supported on $\partial\Theta$. If ϕ is a smooth test function supported on a set $B_r(x)$, a small neighborhood of $x \in \partial A$, then we have

$$\langle Lq, \phi \rangle = \int_{\mathbb{R}^d} q(x)L^*\phi(x)\, \mathrm{d}x$$

$$= \int_{B_r(x)\cap\Theta} Lq(x)\phi(x)\, \mathrm{d}x + \int_{(\partial A)\cap B_r(x)} \left(q\widehat{n} \cdot \mathrm{div}(a\phi) - (\widehat{n} \cdot a\nabla q)\phi \right)$$

$$+ q\widehat{n} \cdot b\,\phi \Big)\, \mathrm{d}\sigma_A(x)$$

where $\widehat{n}(x)$ is the unit normal vector exterior to Θ, and $d\sigma_A$ is the surface measure on ∂A. Since $q = 0$ on ∂A and $Lq = 0$ on Θ, this implies,

$$\langle Lq, \phi \rangle = - \int\limits_{(\partial A) \cap B_r(x)} \phi \, \widehat{n} \cdot a \nabla q \, d\sigma_A(x).$$

That is (after a similar calculation for points on ∂B),

$$Lq(x) = -\widehat{n}(x) \cdot a(x) \nabla q(x) \, d\sigma_A(x) - \widehat{n}(x) \cdot a(x) \nabla q(x) \, d\sigma_B(x), \qquad (1.19)$$

in the sense of distributions. Restricting on ∂A, we get

$$\eta_A = -\rho(x)\widehat{n}(x) \cdot a(x)\nabla q(x) \, d\sigma_A(x). \qquad (1.20)$$

By switching the role of A and B in the above discussion, it is also natural to define a measure on ∂B as

$$\eta_B = \rho(x)\widehat{n}(x) \cdot a(x)\nabla q(x) \, d\sigma_B(x). \qquad (1.21)$$

Note that $1 - q$ gives the forward committor function for the transition from B to A and that $Lq(x) = \eta_A(dx) - \eta_B(dx)$. Although the distributions η_A and η_B are positive (by (1.9)), they need not be probability distributions. Nevertheless, the mass of the two measures is the same.

Lemma 1.3 *The measures η_A and η_B satisfy $\eta_A(\partial A) = \eta_B(\partial B)$. That is,*

$$\int\limits_{\partial A} \rho(x)\widehat{n}(x) \cdot a(x)\nabla q(x) \, d\sigma_A(x) + \int\limits_{\partial B} \rho(x)\widehat{n}(x) \cdot a(x)\nabla q(x) \, d\sigma_B(x) = 0. \quad (1.22)$$

This computation motivates us to define

$$\eta_A^-(dx) = \frac{1}{\nu}\eta_A(dx) = -\frac{1}{\nu}\rho(x)\widehat{n}(x) \cdot a(x)\nabla q(x) \, d\sigma_A(x), \qquad (1.23)$$

$$\eta_B^-(dx) = \frac{1}{\nu}\eta_B(dx) = \frac{1}{\nu}\rho(x)\widehat{n}(x) \cdot a(x)\nabla q(x) \, d\sigma_B(x), \qquad (1.24)$$

We call these distributions the **reactive exit distribution** on ∂A and on ∂B, respectively. The constant ν is a normalizing constant so that η_A^- and η_B^- define probability measures on ∂A and ∂B. By Lemma 1.3, the normalizing constant is the same for both measures. Our next result relates the reactive exit distribution on ∂A to the **empirical reactive exit distribution** on ∂A, defined by

$$\mu_{A,N}^- = \frac{1}{N}\sum_{k=0}^{N-1} \delta_{X_{\tau_{A,k}^-}}(x). \qquad (1.25)$$

Proposition 1.4 *Let $\mu_{A,N}^-$ be the empirical reactive exit distribution on ∂A defined by (1.25). Then $\mu_{A,N}^-$ converges weakly to η_A^- as $N \to \infty$. That is, for any continuous and bounded $f : \partial A \to \mathbb{R}$*

$$\lim_{N \to \infty} \int_{\partial A} f(x)\, d\mu_{A,N}^-(x) = \int_{\partial A} f(x)\, d\eta_A^-(x)$$

holds $\mathbb{P}$-almost surely.

A similar statement holds for the reactive exit distribution on ∂B and the empirical distribution of the points $X_{\tau_{B,k}^-}$. The reactive exit distribution $\eta_A^-(dx)$ is related to the equilibrium measure $e_{A,B}(dx)$ in the potential theory for diffusion processes [7,8], [32, Section 2.3]. In fact, the committor function q is known as the equilibrium potential in those works, and the equilibrium measure $e_{A,B}(dx)$ is given by Lq restricted on ∂A (see equation (2.11) of [7]). Specifically, we have

$$\eta_A^-(dx) = \frac{1}{\nu} \rho(x) e_{A,B}(dx). \tag{1.26}$$

The reactive exit distribution was also used in the milestoning algorithm as in [35]. To the best of our knowledge, Proposition 1.4 for the first time characterizes the equilibrium measure from a dynamic perspective. In the case that the drift $b(x) = -\nabla V(x)$ is a gradient field and $\sigma = \sqrt{\epsilon} I$ is a multiple of the identity matrix, the constant ν is related to the capacity of the sets A and B:

$$\nu = Z^{-1} \mathrm{cap}_A(B), \quad Z = \int_{\mathbb{R}^d} e^{-V(x)/\epsilon}\, dx.$$

(See definition (2.13) of [7] for $\mathrm{cap}_A(B)$.) The results we present here do not require that $b(x)$ is a gradient field; nevertheless, the constant ν still admits the integral representation given below in Proposition 1.8.

We also identify the limit of the **empirical reactive entrance distribution** on ∂B, defined as

$$\mu_{B,N}^+ = \frac{1}{N} \sum_{k=0}^{N-1} \delta_{X_{\tau_{B,k}^+}}(x). \tag{1.27}$$

To describe its limit as $N \to \infty$, let us denote by $\widetilde{L}$ the adjoint of L in $L^2(\mathbb{R}^d, \rho(x)dx)$, given by

$$\widetilde{L}u = -b \cdot \nabla u + \frac{2}{\rho} \mathrm{div}(a\rho) \cdot \nabla u + \mathrm{tr}(a\nabla^2 u). \tag{1.28}$$

This corresponds to the generator of the time-reversed process $t \mapsto X_{T-t}$ [19]. Note that $\widetilde{L} = L$ if the SDE (1.1) is reversible, *i.e.* L is self-adjoint in $L^2(\mathbb{R}^d, \rho(x)\, dx)$. In addition to the forward committor function $q(x)$ (recall (1.7)), we also define the **backward committor function** $\widetilde{q}(x)$ to be the unique solution of

$$\widetilde{L}\widetilde{q} = 0, \quad x \in \Theta$$

with boundary condition

$$\widetilde{q}(x) = \begin{cases} 1, & x \in \partial A \\ 0, & x \in \partial B. \end{cases}$$

In terms of $\widetilde{q}$, we define the **reactive entrance distribution** on ∂B as

$$\eta_B^+(dx) = -\frac{1}{\nu}\rho(x)\widehat{n}(x) \cdot a(x)\nabla\widetilde{q}(x)\, d\sigma_B(x) \tag{1.29}$$

and analogously the reactive entrance distribution on ∂A

$$\eta_A^+(dx) = \frac{1}{\nu}\rho(x)\widehat{n}(x) \cdot a(x)\nabla\widetilde{q}(x)\, d\sigma_A(x). \tag{1.30}$$

Again, ν is a normalizing constant so that these are probability measures; ν is the same as the constant in (1.23). The following proposition justifies the definition of the reactive entrance distribution.

Proposition 1.5 *Let $\mu_{B,N}^+$ be the empirical reactive entrance distribution on ∂B defined by (1.27). Then $\mu_{B,N}^+$ converges weakly to η_B^+ as $N \to \infty$. That is, for any continuous and bounded $f : \partial B \to \mathbb{R}$*

$$\lim_{N\to\infty} \int_{\partial B} f(x)\, d\mu_{B,N}^+(x) = \int_{\partial B} f(x)\, d\eta_B^+(x)$$

holds $\mathbb{P}$-almost surely.

A similar statement holds for the reactive entrance distribution on ∂A and the empirical distribution of the points $X_{\tau_{A,k}^+}$.

Remark 1.6 If the SDE (1.1) is reversible, we have $\widetilde{q} = 1 - q$, and hence $\eta_A^+(dx) = \eta_A^-(dx)$ and $\eta_B^+(dx) = \eta_B^-(dx)$.

In view of Proposition 1.4, η_A^- is a natural choice for the distribution of Y_0. With this choice, the transition path process Y_t characterizes the empirical distribution of $A \to B$ reactive trajectories, as the next theorem shows:

Theorem 1.7 *Let X_t satisfy the SDE (1.1). Let Y^k denote the kth $A \to B$ reactive trajectory defined by (1.5). Let Y be the unique process defined by Theorem 1.1 with initial distribution $Y_0 \sim \eta_A^-(dx)$ on ∂A defined by (1.23), and let $\mathcal{Q}_{\eta_A^-}$ denote the law of this process on $\mathcal{X} = C([0, \infty))$. Then for any $F \in L^1(\mathcal{X}, \mathcal{B}, \mathcal{Q}_{\eta_A^-})$, the limit*

$$\lim_{N\to\infty} \frac{1}{N} \sum_{k=0}^{N-1} F(Y^k) = \widehat{\mathbb{E}}[F(Y)]$$

holds $\mathbb{P}$-almost surely.

In particular, the limit $\widehat{\mathbb{E}}[F(Y)]$ is independent of X_0. Using Theorem 1.7, several interesting statistics of the transition paths can be expressed in terms of the quantities we have defined. Actually, Proposition 1.4 is an immediate corollary of Theorem 1.7, by choosing $F(Y^k) = f(Y_0^k)$, so we will not give a separate proof of Proposition 1.4.

1.3 Reaction rate

Let N_T be the number of $A \to B$ reactive trajectories up to time T:

$$N_T = 1 + \max_k \left\{ k \geq 0 \mid \tau_{B,k}^+ \leq T \right\}.$$

The **reaction rate** ν_R is defined by the limit

$$\nu_R = \lim_{T \to \infty} \frac{N_T}{T} = \lim_{k \to \infty} \frac{k}{\tau_{B,k}^+}, \tag{1.31}$$

and it is the rate of the transition from A to B. Also, the limits

$$T_{AB} := \lim_{N \to \infty} \frac{1}{N} \sum_{k=0}^{N-1} \left(\tau_{B,k}^+ - \tau_{A,k}^+ \right) \tag{1.32}$$

and

$$T_{BA} := \lim_{N \to \infty} \frac{1}{N} \sum_{k=0}^{N-1} \left(\tau_{A,k+1}^+ - \tau_{B,k}^+ \right) \tag{1.33}$$

are the **expected reaction times** from $A \to B$ and $B \to A$, respectively. The reaction rate from $A \to B$ and $B \to A$ are then given by $k_{AB} = T_{AB}^{-1}$ and $k_{BA} = T_{BA}^{-1}$. Another interesting quantity is the **expected crossover time** from $A \to B$

$$C_{AB} := \lim_{N \to \infty} \frac{1}{N} \sum_{k=0}^{N-1} \left(\tau_{B,k}^+ - \tau_{A,k}^- \right), \tag{1.34}$$

which is the typical duration of the $A \to B$ reactive intervals. Observe that $C_{AB} < T_{AB}$. Similarly, we define

$$C_{BA} := \lim_{N \to \infty} \frac{1}{N} \sum_{k=0}^{N-1} \left(\tau_{A,k+1}^+ - \tau_{B,k}^- \right). \tag{1.35}$$

The next result identifies these limits in terms of the committor functions and the reactive exit and entrance distributions.

Proposition 1.8 *The limits* (1.31)*,* (1.32)*,* (1.33)*,* (1.34)*, and* (1.35) *hold* $\mathbb{P}$*-almost surely, and*

$$v_R = v = \int_{\mathbb{R}^d} \rho(x) \nabla q(x) \cdot a(x) \nabla q(x) \, dx.$$

$$T_{AB} = \int_{\partial A} \eta_A^+(dx) u_B(x) = \frac{1}{v_R} \int_{\mathbb{R}^d} \rho(x) \widetilde{q}(x) \, dx.$$

$$T_{BA} = \int_{\partial B} \eta_B^+(dx) u_A(x) = \frac{1}{v_R} \int_{\mathbb{R}^d} \rho(x)(1 - \widetilde{q}(x)) \, dx.$$

$$C_{AB} = \int_{\partial A} \eta_A^-(dx) v_B(x) = \frac{1}{v_R} \int_{\mathbb{R}^d} \rho(x) q(x) \widetilde{q}(x) \, dx.$$

$$C_{BA} = \int_{\partial B} \eta_B^-(dx) v_A(x) = \frac{1}{v_R} \int_{\mathbb{R}^d} \rho(x)(1 - q(x))(1 - \widetilde{q}(x)) \, dx.$$

Here $u_B(x) = \mathbb{E}[\tau_B^X \mid X_0 = x]$ *is the mean first hitting time of* X_t *to* $\overline{B}$, *and* $v_B(x) = \widehat{\mathbb{E}}[\tau_B^Y \mid Y_0 = x]$ *is the mean first hitting time of* Y_t *to* $\overline{B}$. *Similarly, if* q *is replaced by* $(1-q)$ *in the definition of* Y, *then* $v_A(x) = \widehat{\mathbb{E}}[\tau_A^Y \mid Y_0 = x]$. *Recall that* v *is the normalizing factor for the reactive exit and entrance distributions.*

The formulas for v_R, T_{AB}, and T_{BA} were obtained in [15]. We believe the formulas for C_{AB} and C_{BA} are new. We also note that the crossover time for the transition path process in one dimension was recently studied in [4,10] by other methods.

1.4 Density of transition paths

We now consider the distribution ρ_R as defined in [15]:

$$\rho_R(z) = \lim_{T \to \infty} \frac{1}{T} \int_0^T \delta(z - X_t) \mathbb{I}_R(t) \, dt, \quad z \in \Theta, \tag{1.36}$$

where R is the random set of times at which X_t is reactive:

$$R = \bigcup_{k=0}^{\infty} [\tau_{A,k}^-, \tau_{B,k}^+].$$

This distribution on Θ can be viewed as the density of transition paths. By Proposition 1.8, and Theorem 1.7, we can describe ρ_R in terms of the transition density for Y_t. Specifically, for any continuous and bounded function $f : \mathbb{R}^d \to \mathbb{R}$, we have

$$\int_\Theta f(z)\rho_R(z)\,dz = \nu_R \lim_{T\to\infty} \frac{1}{N_T} \int_0^T f(X_t)\mathbb{I}_R(t)\,dt$$

$$= \nu_R \lim_{N\to\infty} \frac{1}{N} \sum_{k=0}^{N-1} \int_0^{\tau_{B,k}^+ - \tau_{A,k}^-} f\left(Y_t^k\right)\,dt$$

$$= \nu_R \widehat{\mathbb{E}} \left[\int_0^{t_B} f(Y_t)\,dt \mid Y_0 \sim \eta_A^- \right]$$

$$= \nu_R \int_0^\infty \int_\Theta Q_R(t, \eta_A^-, z) f(z)\,dz\,dt.$$

Here $Q_R(t, \eta_A^-, z)$ is the density of Y_t, with $Y_0 \sim \eta_A^-$, and killed at ∂B

$$Q_R(t, \eta_A^-, z) = \mathbb{Q}(Y_t \in dz,\ t < t_B \mid Y_0 \sim \eta_A^-), \tag{1.37}$$

and t_B is the first hitting time of Y_t to $\overline{B}$. Hence, for $z \in \Theta$,

$$\rho_R(z) = \nu_R \int_0^\infty Q_R(t, \eta_A^-, z)\,dt. \tag{1.38}$$

Proposition 1.9 *For all $z \in \Theta$,*

$$\rho_R(z) = \rho(z)q(z)\widetilde{q}(z). \tag{1.39}$$

This formula for ρ_R was first derived in [15,22].

1.5 Current of transition paths

The density $Q_R(t, \eta_A^-, z)$ satisfies the adjoint equation

$$\frac{\partial}{\partial t} Q_R(t, \eta_A^-, z) = (L^q)^* Q_R(t, \eta_A^-, z), \quad z \in \Theta$$

where $(L^q)^*$ is the adjoint of L^q:

$$(L^q)^* u = \sum_{i,j} (a_{ij}(z)u(z))_{z_i z_j} - \sum_i (K_i(z)u(z))_{z_i}$$

and K is defined by (1.13). Integrating from $t = 0$ to $t = \infty$ we see that $\rho_R(z)$ satisfies

$$(L^q)^* \rho_R(z) = 0, \quad z \in \Theta.$$

In divergence form, this equation is

$$\nabla_z \cdot J_R(z) = 0, \tag{1.40}$$

where the vector field

$$\begin{aligned}
J_R(z) &= \rho_R(z)\left(b(z) - \frac{2a\nabla q(z)}{q(z)}\right) + \mathrm{div}(a(z)\rho_R(z)) \\
&= \Big(b(z)\rho(z) - \mathrm{div}\big(a(z)\rho(z)\big)\Big)q(z)\widetilde{q}(z) \\
&\quad - \rho(z)a(z)\Big(\widetilde{q}(z)\nabla q(z) - q(z)\nabla\widetilde{q}(z)\Big).
\end{aligned} \tag{1.41}$$

is continuous over $\overline{\Theta}$. The vector field $J_R(z)$, identified in [15], may be regarded as the **current of transition paths** (see Remark 1.13). Observe that if the SDE (1.1) is reversible, we have $\widetilde{q} = 1 - q$ and

$$b(z)\rho(z) - \mathrm{div}(a(z)\rho(z)) = 0,$$

and hence the current given by (1.41) simplifies to

$$J_R(z) = \rho(z)a(z)\nabla q(z).$$

This was observed already in [15]. The current was also discussed in potential theory in the context of reversible Markov chains, see e.g. [9].

On the boundary, the current (1.41) is related to the reactive exit and entrance distributions.

Proposition 1.10 *We have*

$$J_R = \rho a\nabla q \ on \ \partial A, \quad and \quad J_R = -\rho a\nabla\widetilde{q}, \ on \ \partial B,$$

and hence,

$$\eta_A^-(\mathrm{d}x) = -v_R^{-1}\widehat{n}(x)\cdot J_R(x)\,\mathrm{d}\sigma_A(x) \quad and \quad \eta_B^+(\mathrm{d}x) = v_R^{-1}\widehat{n}(x)\cdot J_R(x)\,\mathrm{d}\sigma_B(x).$$

As an immediate corollary, we have an additional formula for the reaction rate.

Corollary 1.11 *Let S be a set with smooth boundary that contains A and separates A and B, we have*

$$v_R = \int_{\partial S} \widehat{n}(x)\cdot J_R(x)\,\mathrm{d}\sigma_S(x), \tag{1.42}$$

where $\widehat{n}$ is the unit normal vector exterior to S.

The current J_R generates a (deterministic) flow in $\overline{\Theta}$ stopped at ∂B:

$$\frac{\mathrm{d}Z_t^z}{\mathrm{d}t} = J_R(Z_t^z), \quad \text{for } 0 \le t \le t_B, \quad Z_0^z = z \tag{1.43}$$

where $t_B = t_B(z)$ is the time at which Z_t reaches ∂B. As J_R is divergence free in Θ, $J_R \cdot \widehat{n} < 0$ on ∂A, and $J_R \cdot \widehat{n} > 0$ on ∂B, $t_B(z)$ is finite for any $z \in \overline{\Theta}$. The flow naturally defines a map $\Phi_{J_R} : \partial A \to \partial B$: given any point $z \in \partial A$, we define

$$\Phi_{J_R}(z) = Z^z_{t_B} \in \partial B. \tag{1.44}$$

Proposition 1.12 *For any $f \in C^1(\mathbb{R}^d)$,*

$$\int\limits_{\partial B} f(x)\eta_B^+(dx) - \int\limits_{\partial A} f(x)\eta_A^-(dx) = \frac{1}{\nu_R} \int\limits_{\Theta} J_R \cdot \nabla f \, dx. \tag{1.45}$$

In particular,

$$\Phi_{J_R,*}(\eta_A^-) = \eta_B^+,$$

where $\Phi_{J_R,*}(\eta_A^-)$ is the pushforward of the measure η_A^- by the map Φ_{J_R}.

Hence, J_R characterizes "the flow of reactive trajectories" from A to B.

Remark 1.13 Note that by Propositions 1.4 and 1.5, the left hand side of (1.45) is equal, $\mathbb{P}$-almost surely, to the limit

$$\lim_{N \to \infty} \frac{1}{N} \sum_{n=0}^{N-1} \left(f(X_{\tau_{B,n}^+}) - f(X_{\tau_{A,n}^-}) \right).$$

If X_t was differentiable, we would have

$$\lim_{N \to \infty} \frac{1}{N} \sum_{n=0}^{N-1} \left(f(X_{\tau_{B,n}^+}) - f(X_{\tau_{A,n}^-}) \right) = \lim_{T \to \infty} \frac{1}{\nu_R} \frac{1}{T} \int\limits_0^T 1_R(t) \frac{d}{dt} f(X_t) \, dt$$

$$\text{``} = \frac{1}{\nu_R} \int\limits_{\Theta} dx \nabla f(x) \cdot \lim_{T \to \infty} \frac{1}{T} \int\limits_0^T \dot{X}_t \delta(x - X_t) 1_R(t) \, dt \text{ '',}$$

Combining this with Proposition 1.12, we arrive at a formal characterization of J_R

$$J_R \text{``} = \lim_{T \to \infty} \frac{1}{T} \int\limits_0^T \dot{X}_t \delta(x - X_t) 1_R(t) \, dt \text{ '',}$$

This formal expression was used in [15] to define J_R.

1.6 Related work

As we have mentioned, our work is closely related to the transition path theory developed by Weinan and Vanden-Eijnden [15,16,24], which is a framework for studying

the transition paths. In particular, based on the committor function, formula for reaction rate, density and current of transition paths were obtained in [15]. Our main motivation is to understand the probability law of the transition paths. The main results Theorems 1.1, 1.2, and 1.7 identify an SDE which characterizes the law of the transition paths in $C([0, \infty))$. Therefore, as an application of these results, we are able to give rigorous proofs for the formula for reaction rate, density and current of transition paths in [15]. We note that in the discrete case, a generator analogous to (1.10) was also proposed very recently in [33] for Markov jumping processes.

Our results may be useful in the design of numerical path-sampling algorithms. Specifically, the results indicate that with knowledge of the committor function $q(x)$ one can bias the sampling of X_t in order to directly sample the reactive trajectories, without an acceptance/rejection procedure. Of course, this assumes knowledge of the committor function, which is certainly non-trivial as it involves solving a high dimensional PDE; $q(x)$ is explicit only in the simplest of cases (such as when $d = 1$). We refer to [16,27] and references therein for efforts in numerical approximations of committor functions. Nevertheless, our theoretical results might be used to analyze methods of sampling reactive trajectories. In particular, it would be important to know what sort of approximation of q could be used to efficiently sample the reactive trajectories. This issue is related to importance sampling algorithms for rare events (see e.g. [13,36]). We plan to explore these issues more in future works.

The transition paths start at ∂A and terminate at ∂B, and hence they can be viewed as paths of a bridge process between $\overline{A}$ and $\overline{B}$. In this perspective, our work is related to the conditional path sampling for SDEs studied in [20,21,29,31]. In those works, stochastic partial differential equations were proposed to sample SDE paths with fixed end points. However, the paths considered were different from the transition paths as their time duration is fixed a priori. It would be interesting to explore SPDE-based sampling strategies for the transition path process identified in Theorem 1.1.

Let us also point out that in the work we present here we do not assume that the noise σ is small, as is the case in the asymptotic results of [7,8,10], which we have mentioned already, and also in some other works, such as the large deviation theory of Freidlin and Wentzell [17].

After this paper was submitted for publication, both Sznitman and one of the editors brought to our attention the relevant work of Meyer et al. [25]. If we define the non-decreasing processes

$$V_t^A = \# \left\{ k \in \mathbb{Z}^+ \mid \tau_{A,k}^+ \le t \right\},$$
$$V_t^B = \# \left\{ k \in \mathbb{Z}^+ \mid \tau_{B,k}^+ \le t \right\},$$

where $\mathbb{Z}^+$ is the set of non-negative integers, then the triple (X_t, V_t^A, V_t^B) is a Markov process on $\mathbb{R}^d \times \mathbb{Z}^+ \times \mathbb{Z}^+$. Moreover, the exit times $\tau_{A,k}^-$ defined above coincide with the random times $L_k = \sup\{t \ge 0 \mid (X_t, V_t^A, V_t^B) \in \overline{A} \times \{k+1\} \times \{k\}\}$. Although it is not a stopping time, L_k is a coterminal time, as defined in [25]. Theorem 5.1 of [25] applied to $(X_{t+L_k}, V_{t+L_k}^A, V_{t+L_k}^B)$ then implies that for $t > 0$, Y_t^k is a strong Markov process with transition probability (1.11). In particular, this implies that for any $t_0 > 0$ and any bounded and continuous functional $F : C([t_0, \infty)) \to \mathbb{R}$, we have

$$\mathbb{E}[F(Y_t^k, t \geq t_0)] = \widehat{\mathbb{E}}\big[F(Y_t, t \geq t_0) \mid Y_{t_0} = Y_{t_0}^k\big].$$

This is similar to but weaker than the statement of Theorem 1.2, which also applies to $t_0 = 0$. Moreover, the results of [25] do not identify the reactive exit distribution, which plays an important role in Theorem 1.7.

The rest of the paper is organized as follows. Theorems 1.1 and 1.2 are proved in Sect. 2. In Sect. 3 we prove Lemma 1.3, Proposition 1.5 and Theorem 1.7 related to the reactive entrance and exit distributions. As we have mentioned, Proposition 1.4 follows immediately from Theorem 1.7, so we do not give a separate proof of it. Propositions 1.8, 1.9, 1.10, Corollary 1.11, and Proposition 1.12 are proved in Sect. 4.

2 The transition path process

Proof of Theorem 1.1 Without loss of generality, we prove the theorem in the case that $\xi \equiv y_0$ is a single point in $\overline{\Theta}$. The interesting aspect of the theorem is that y_0 is allowed to be on $\partial\Theta$, since the drift term is singular at $\partial\Theta$. If we assume that $y_0 \in \Theta$, then existence of a unique strong solution up to the time $\tau_A \wedge \tau_B$ follows from standard arguments, since $K(y)$ is Lipschitz continuous in the interior of Θ. That is, if $y_0 \in \Theta$, there is a unique, continuous $\widehat{\mathcal{F}}_t$-adapted process Y_t which satisfies

$$Y_t = y_0 + \int_0^{t \wedge (\tau_A \wedge \tau_B)} K(Y_s)\, \mathrm{d}s + \int_0^{t \wedge (\tau_A \wedge \tau_B)} \sqrt{2}\,\sigma(Y_s)\, \mathrm{d}\widehat{W}_s, \quad t \geq 0. \tag{2.1}$$

Moreover, if $y_0 \in \Theta$, then we must have $\tau_A > \tau_B > 0$ almost surely. This follows from an argument similar to the proof of [23, Proposition 3.3.22, p. 161]. Specifically, we consider the process $z_t = 1/q(Y_t) \in \mathbb{R}$, which satisfies

$$z_{t \wedge \tau} = z_0 - \int_0^{t \wedge \tau} \sqrt{2}(z_s)^2 \nabla q \cdot \sigma\, \mathrm{d}\widehat{W}_s$$

where $\tau = \tau_B \wedge \tau_\epsilon$ with $\tau_\epsilon = \inf\{t > 0 \mid q(Y_t) = \epsilon\}$. Since $\tau < \infty$ with probability one, we have

$$z_0 = \widehat{\mathbb{E}}[z_{t \wedge \tau}] = \frac{1}{q(\epsilon)}\mathbb{Q}(\tau_\epsilon < \tau_B) + \mathbb{Q}(\tau_\epsilon > \tau_B).$$

Hence $\mathbb{Q}(\tau_\epsilon < \tau_B) \leq q(\epsilon)(z_0 - 1)$. So, $\mathbb{Q}(\tau_A < \tau_B) \leq \lim_{\epsilon \to 0} \mathbb{Q}(\tau_\epsilon < \tau_B) = 0$.

Now suppose $y_0 \in \partial A$. In consideration of the comments above, it suffices to prove the desired result with τ_B replaced by τ_r, the first hitting time to $\partial B_r(y_0) \cap \Theta$, where $B_r(y_0)$ is a ball of radius $r > 0$ centered at y_0. Thus, we want to prove existence and pathwise uniqueness of a continuous $\widehat{\mathcal{F}}_t$-adapted process $Y_t : [0, \infty) \to \overline{\Theta}$ satisfying

$$Y_t = y_0 + \int_0^{t \wedge \tau_r} K(Y_s) \, ds + \int_0^{t \wedge \tau_r} \sqrt{2} \, \sigma(Y_s) \, d\widehat{W}_s, \qquad (2.2)$$

where

$$\tau_r = \inf \{t \geq 0 \mid Y_t \in \partial B_r(y_0) \cap \Theta\}.$$

It will be very useful to define a new coordinate system in the set $B_r^+(y_0) = B_r(y_0) \cap \Theta$ and to consider the problem in these new coordinates. For $r > 0$ small enough we can define a C^3 map $(h^{(1)}(y), \ldots, h^{(d-1)}(y), q(y)) : \overline{B_r^+(y_0)} \to \mathbb{R}^{d-1} \times [0, \infty)$, such that the scalar functions $h^{(i)}(y) : \overline{B_r^+(y_0)} \to \mathbb{R}$ satisfy

$$\langle \nabla h^{(i)}(y), a(y) \nabla q(y) \rangle = 0, \quad \forall \, y \in \overline{B_r^+(y_0)}, \qquad i = 1, \ldots, d-1. \qquad (2.3)$$

Furthermore, the map may be constructed so that it is invertible on its range and that the inverse is C^3. The existence of such a map follows from the regularity of ∂A, the regularity of q, and the fact that $\langle \widehat{n}, a \nabla q \rangle \neq 0$ on ∂A by (1.9).

For two initial points $x_1, x_2 \in \Theta$, let $Y_t^{x_1}$ and $Y_t^{x_2}$ denote the unique solutions to (2.1) with $Y_0^{x_1} = x_1$ and $Y_0^{x_2} = x_2$ respectively. That is,

$$Y_t^x = x + \int_0^{t \wedge \tau_B^x} K(Y_s^x) \, ds + \int_0^{t \wedge \tau_B^x} \sqrt{2} \, \sigma(Y_s^x) \, d\widehat{W}_s, \quad t \geq 0, \qquad (2.4)$$

where τ_B^x is the first hitting time of Y_t^x to ∂B. Changing to the coordinate system defined by $(h^{(1)}(y), \ldots, h^{(d-1)}(y), q(y))$, we denote

$$(h_{1,t}, q_{1,t}) = (h(Y_t^{x_1}), q(Y_t^{x_1})) \quad \text{and} \quad (h_{2,t}, q_{2,t}) = (h(Y_t^{x_2}), q(Y_t^{x_2})).$$

Let τ_r^1 and τ_r^2 denote the first hitting times of $Y_t^{x_1}$ and $Y_t^{x_2}$ to the set $\partial B_r(y_0) \cap \Theta$. The processes $(h_{1,t}, q_{1,t})$ and $(h_{2,t}, q_{2,t})$ are well-defined up to the times τ_r^1 and τ_r^2, respectively.

We can control the difference between $(h_{1,t}, q_{1,t})$ and $(h_{2,t}, q_{2,t})$:

Lemma 2.1 *There is a constant C such that for all $x_1, x_2 \in B_{r/2}(y_0) \cap \Theta$*

$$\widehat{\mathbb{E}} \left[\max_{t \in [0,T]} (q_{1,t \wedge \tau} - q_{2,t \wedge \tau})^2 \right] \leq C |x_1 - x_2|^{1/2},$$

and

$$\widehat{\mathbb{E}} \left[\max_{t \in [0,T]} |h_{1,t \wedge \tau} - h_{2,t \wedge \tau}|^2 \right] \leq C |x_1 - x_2|,$$

where $\tau = \tau_r^1 \wedge \tau_r^2$.

The proof of Lemma 2.1 will be postponed. One immediate corollary is the following.

Corollary 2.2 *There is a constant C such that for all $x_1, x_2 \in B_{r/2}(y_0) \cap \Theta$*

$$\mathbb{Q}\left(\max_{0 \leq t \leq (T \wedge \tau)} |Y_t^{x_1} - Y_t^{x_2}| > \alpha\right) \leq C\alpha^{-2}|x_1 - x_2|^{1/2}, \quad \forall \alpha > 0, \tag{2.5}$$

where $\tau = \tau_r^1 \wedge \tau_r^2$.

Proof On the closed set $\{z \in \mathbb{R}^d \mid z = (h(y), q(y)), \ y \in \overline{B_r^+(y_0)}\}$, the map $y \mapsto (h(y), q(y))$ is invertible with a continuously differentiable inverse. Hence there is a constant C, depending only on the map $y \mapsto (h(y), q(y))$ such that

$$|Y_t^{x_1} - Y_t^{x_2}| \leq C \left(|h_{1,t} - h_{2,t}| + |q_{1,t} - q_{2,t}|\right), \quad \forall t \in [0, \tau].$$

By combining this bound with Chebychev's inequality and Lemma 2.1 we obtain (2.5). □

Now suppose $y_0 \in \partial A$. Let $\{x_n\}_{n=1}^{\infty} \subset \Theta$ be a given sequence such that $x_n \to y_0$ as $n \to \infty$. For each n, define $Y_t^{x_n}$ by (2.4), and let τ_r^n denote the first hitting time of $Y_t^{x_n}$ to $\partial B_r(y_0) \cap \Theta$. We may choose the points x_n so that $|x_n - y_0| \leq 25^{-n}$. Define $\widehat{\tau}^n = \tau_r^{n+1} \wedge \tau_r^n$. Applying Corollary 2.2, we conclude

$$\mathbb{Q}\left(\max_{0 \leq t \leq (T \wedge \widehat{\tau}^n)} |Y_t^{x_{n+1}} - Y_t^{x_n}| > 2^{-n}\right) \leq C2^{2n}5^{-n}.$$

Therefore, by the Borel–Cantelli lemma, the series

$$\sum_{n=1}^{\infty} \max_{0 \leq t \leq (T \wedge \widehat{\tau}^n)} |Y_t^{x_{n+1}} - Y_t^{x_n}| < \infty \tag{2.6}$$

with probability one. Let us define

$$\tau_r = \liminf_{n \to \infty} \tau_r^n = \liminf_{n \to \infty} \widehat{\tau}^n. \tag{2.7}$$

We will prove that τ_r is positive:

Lemma 2.3 *For all $r > 0$ sufficiently small, $\mathbb{Q}(\tau_r > 0) = 1$.*

In view of (2.6) and Lemma 2.3, we conclude that there must be a continuous process Y_t such that, with probability one,

$$Y_t^{x_n} \to Y_t$$

uniformly on compact subsets of $[0, \tau_r)$, as $n \to \infty$. Let us define

$$\overline{\tau}_{r/2} = \inf\{t \geq 0 \mid Y_t \in \partial B_{r/2}(y_0) \cap \Theta\}. \tag{2.8}$$

Lemma 2.4 *For all $r > 0$ sufficiently small, $\mathbb{Q}(\overline{\tau}_{r/2} \in (0, \tau_r)) = 1$, and $\overline{\tau}_{r/2}$ is stopping time with respect to $\widehat{\mathcal{F}}_t$.*

We will postpone the proof of Lemmas 2.3 and 2.4. Since $\overline{\tau}_{r/2} < \tau_r$, $Y_t^{x_n} \to Y_t$ uniformly on $[0, \overline{\tau}_{r/2}]$. Let us now replace Y_t by the stopped process $Y_{t \wedge \overline{\tau}_{r/2}}$. Since each $Y_t^{x_n}$ is $\widehat{\mathcal{F}}_t$-adapted, so is the limit Y_t. We claim that Y_t satisfies

$$Y_t = y_0 + \int_0^{t \wedge \overline{\tau}_{r/2}} K(Y_s) \, ds + \int_0^{t \wedge \overline{\tau}_{r/2}} \sqrt{2} \, \sigma(Y_s) \, d\widehat{W}_s, \quad t \geq 0. \tag{2.9}$$

Since $Y_t^{x_n} \to Y_t$ uniformly on $[0, \overline{\tau}_{r/2}]$, we have $(q(Y_t^{x_n}), h(Y_t^{x_n})) \to (q(Y_t), h(Y_t))$ uniformly on $[0, \overline{\tau}_{r/2}]$, and $(q_t, h_t) = (q(Y_t), h(Y_t))$ satisfies

$$h_t = h_0 + \int_0^{t \wedge \overline{\tau}_{r/2}} f(q_s, h_s) \, ds + \int_0^{t \wedge \overline{\tau}_{r/2}} m(q_s, h_s) \, d\widehat{W}_s, \tag{2.10}$$

and

$$q_t - \int_0^{t \wedge \overline{\tau}_{r/2}} g(q_s, h_s) \cdot d\widehat{W}_s = \lim_{n \to \infty} \int_0^{t \wedge \tau_r^n} \frac{|g(q_s^{x_n}, h_s^{x_n})|^2}{q_s^{x_n}} \, ds. \tag{2.11}$$

for all $t \in [0, \overline{\tau}_{r/2}]$, where $(q_t^{x_n}, h_t^{x_n}) = (q(Y_t^{x_n}), h(Y_t^{x_n}))$. (Recall $q_0 = 0$.) Since $q_s^{x_n} > 0$, the last limit can be bounded below using Fatou's lemma:

$$q_t - \int_0^{t \wedge \overline{\tau}_{r/2}} g(q_s, h_s) \cdot d\widehat{W}_s \geq \int_0^{t \wedge \overline{\tau}_{r/2}} \liminf_{n \to \infty} \frac{|g(q_s^{x_n}, h_s^{x_n})|^2}{q_s^{x_n}} \, ds = \int_0^{t \wedge \overline{\tau}_{r/2}} \frac{|g(q_s, h_s)|^2}{q_s} \, ds. \tag{2.12}$$

Recall that $|g(q_s, h_2)|^2 \geq C_r > 0$. In particular, with probability one, the random set $H = \{s \in [0, \overline{\tau}_{r/2}] \mid q_s = 0\}$ must have zero Lebesgue measure; if that were not the case, then we would have

$$- \int_0^{t \wedge \overline{\tau}_{r/2}} g(q_s, h_s) \cdot d\widehat{W}_s = +\infty,$$

for all t in a set of positive Lebesgue measure, an event which happens with zero probability. Therefore, by Fubini's theorem,

$$0 = \widehat{\mathbb{E}} \int_0^T \mathbb{I}_H(s) \, ds = \int_0^T \mathbb{Q}(s < \overline{\tau}_{r/2}, \, q_s = 0) \, ds$$

which implies that $\mathbb{Q}(s < \overline{\tau}_{r/2}, \ q_s = 0) = 0$ for almost every $s \geq 0$. Since $\overline{\tau}_{r/2} > 0$ almost surely, this implies that we may choose a deterministic sequence of times $t_n \in (0, 1/n]$ such that, almost surely, $q_{t_n} > 0$ for n sufficiently large. By then applying the same argument as when $y_0 \in \Theta$, we conclude that $q_t > 0$ for all $t > t_n$. Hence, $q_t > 0$ for all $t > 0$ must hold with probability one.

Since q_t is continuous, we now know that for any $\epsilon > 0$,

$$\min_{t > \epsilon} q_t > 0.$$

holds with probability one. In particular,

$$\liminf_{n \to \infty} \min_{t > \epsilon} q_t^{x_n} > 0,$$

so that

$$\lim_{n \to \infty} \int_\epsilon^{t \wedge \tau^n} \frac{|g(q_s^{x_n}, h_s^{x_n})|^2}{q_s^{x_n}} \, ds = \int_\epsilon^{t \wedge \overline{\tau}_{r/2}} \frac{|g(q_s, h_s)|^2}{q_s} \, ds,$$

almost surely. Since q_t is continuous at $t = 0$, we also know that

$$\lim_{\epsilon \to 0} \lim_{n \to \infty} \int_0^{t \wedge \tau^n \wedge \epsilon} \frac{|g(q_s^{x_n}, h_s^{x_n})|^2}{q_s^{x_n}} \, ds = \lim_{\epsilon \to 0} \left(q_\epsilon - \int_0^{t \wedge \overline{\tau}_{r/2} \wedge \epsilon} g(q_s, h_s) \cdot d\widehat{W}_s \right) = 0$$

almost surely. Returning to (2.11) we now conclude that

$$
\begin{aligned}
q_t - \int_0^{t \wedge \overline{\tau}_{r/2}} g(q_s, h_s) \cdot d\widehat{W}_s &= \lim_{\epsilon \to 0} \lim_{n \to \infty} \int_0^{t \wedge \tau^n \wedge \epsilon} \frac{|g(q_s^{x_n}, h_s^{x_n})|^2}{q_s^{x_n}} \, ds \\
&\quad + \lim_{\epsilon \to 0} \lim_{n \to \infty} \int_\epsilon^{t \wedge \tau^n} \frac{|g(q_s^{x_n}, h_s^{x_n})|^2}{q_s^{x_n}} \, ds \\
&= \lim_{\epsilon \to 0} \int_\epsilon^{t \wedge \overline{\tau}_{r/2}} \frac{|g(q_s, h_s)|^2}{q_s} \, ds \\
&= \int_0^{t \wedge \overline{\tau}_{r/2}} \frac{|g(q_s, h_s)|^2}{q_s} \, ds \qquad (2.13)
\end{aligned}
$$

holds with probability one. Equation (2.9) for Y_t now follows from (2.10) and (2.13) by changing coordinates.

Except for the proofs of Lemmas 2.1, 2.3, and 2.4, we have now established existence of a strong solution Y_t to (2.2) (with r replaced by $r/2$). The uniqueness of the solution follows by the same arguments. Suppose that Y_t^1 and Y_t^2 both solve (2.2) with the same Brownian motion and the same initial point $Y_0^1 = Y_0^2 = y_0$. Then Corollary 2.2 implies that, $\mathbb{Q}$ almost surely, $Y_t^1 = Y_t^2$ for all $t \in [0, \tau_r^1 \wedge \tau_r^2]$ where τ_r^1 and τ_r^2 are the corresponding hitting times to $\partial B_r(y_0) \cap \Theta$. In particular, $\tau_r^1 = \tau_r^2$. This proves pathwise uniqueness. □

We now prove Lemmas 2.1, 2.3 and 2.4 to complete the proof of Theorem 1.1.

Proof of Lemma 2.1 By Itô's formula the process $(h_1, q_1) = (h_{1,t}, q_{1,t})$ satisfies

$$dh_1 = f(q_1, h_1)\,dt + m(q_1, h_1)\,d\widehat{W}_t, \tag{2.14}$$

$$dq_1 = \frac{|g(q_1, h_1)|^2}{q_1}\,dt + g(q_1, h_1)\cdot d\widehat{W}_t, \tag{2.15}$$

for $0 \le t \le \tau_r^1$, where the functions $g = \sqrt{2}(\nabla q)^{\mathrm{T}}\sigma \in \mathbb{R}^d$, $f = Lh \in \mathbb{R}^{d-1}$, and $m = \sqrt{2}(\nabla h)^{\mathrm{T}}\sigma \in \mathbb{R}^{(d-1)\times d}$, are all Lipschitz continuous in their arguments over $\overline{B_r^+}$. Similarly, $(h_2, q_2) = (h_{2,t}, q_{2,t})$ satisfies

$$dh_2 = f(q_2, h_2)\,dt + m(q_2, h_2)\,d\widehat{W}_t \tag{2.16}$$

$$dq_2 = \frac{|g(q_2, h_2)|^2}{q_2}\,dt + g(q_2, h_2)\cdot d\widehat{W}_t, \tag{2.17}$$

for $0 \le t \le \tau_r^2$. Notice that the choice of coordinates satisfying (2.3) has eliminated a potentially singular drift term in the equations for $h_{1,t}$ and $h_{2,t}$. On the other hand, the drift term in the equations for q_1 and q_2 blows up near the boundary $q = 0$. Indeed, if $r > 0$ is small enough, by (1.9) there is a constant $C_r > 0$ such that

$$\inf_{y \in \overline{B_r^+}} 2\langle \nabla q(y)), a(y)\nabla q(y)\rangle \ge 2\lambda \inf_{y \in \overline{B_r^+}} |\nabla q(y)| \ge C_r. \tag{2.18}$$

Hence,

$$|g(q_{1,t}, h_{1,t})|^2 = 2\langle \nabla q(Y_t^{x_1}), a(Y_t^{x_1})\nabla q(Y_t^{x_1})\rangle \ge 2\lambda \inf_{y \in \overline{B_r^+}} |\nabla q(y)| \ge C_r > 0. \tag{2.19}$$

Letting $\tau = \tau_r^1 \wedge \tau_r^2$ and using (2.14) and (2.16), we compute

$$
\begin{aligned}
d\,|h_1 - h_2|^2 = {} & 2(h_1 - h_2)^{\mathrm{T}}(f(q_1, h_1) - f(q_2, h_2))\,dt \\
& + 2(h_1 - h_2)^{\mathrm{T}}(m(q_1, h_1) - m(q_2, h_2))\,d\widehat{W}_t \\
& + \mathrm{tr}\left((m(q_1, h_1) - m(q_2, h_2))(m(q_1, h_1) - m(q_2, h_2))^{\mathrm{T}}\right)dt
\end{aligned}
$$

for $0 \leq t \leq \tau$. In particular,

$$\widehat{\mathbb{E}}\left[|h_{1,t \wedge \tau} - h_{2,t \wedge \tau}|^2\right] \leq C \int_0^t \widehat{\mathbb{E}}\left[\mathbb{I}_{[0,\tau]}(s)(q_{1,s} - q_{2,s})^2\right] ds$$

$$+C \int_0^t \widehat{\mathbb{E}}\left[\mathbb{I}_{[0,\tau]}(s)|h_{1,s} - h_{2,s}|^2\right] ds + C|x_1 - x_2|,$$

$$\leq C \int_0^t \widehat{\mathbb{E}}\left[(q_{1,s \wedge \tau} - q_{2,s \wedge \tau})^2\right] ds$$

$$+C \int_0^t \widehat{\mathbb{E}}\left[|h_{1,s \wedge \tau} - h_{2,s \wedge \tau}|^2\right] ds + C|x_1 - x_2|,$$

$$(2.20)$$

holds for all $t \geq 0$.

From (2.15) and (2.17) we also compute

$$d(q_1 - q_2)^2 = 2(q_1 - q_2)d(q_1 - q_2) + |g_1 - g_2|^2 dt$$

$$= 2(q_1 - q_2)\left(\frac{|g_1|^2}{q_1} - \frac{|g_2|^2}{q_2}\right) dt$$

$$+2(q_1 - q_2)(g_1 - g_2) \cdot d\widehat{W}_t + |g_1 - g_2|^2 dt \qquad (2.21)$$

for $0 \leq t \leq \tau$, where we have used the notation $g_1 = g(q_1, h_1)$ and $g_2 = g(q_2, h_2)$. We claim that there is a constant C, depending only on r, such that

$$2(q_1 - q_2)\left(\frac{|g_1|^2}{q_1} - \frac{|g_2|^2}{q_2}\right) \leq C(|q_1 - q_2|^2 + |h_1 - h_2|^2) \qquad (2.22)$$

holds for all $t \leq \tau$, with probability one. Both sides of (2.22) are invariant when (q_1, h_1) and (q_2, h_2) are interchanged. So, we may assume $q_1 \leq q_2$ without loss of generality. We consider the following two possibilities. First, suppose that

$$0 \leq q_1 \left||g_1|^2 - |g_2|^2\right| \leq (q_2 - q_1)|g_1|^2. \qquad (2.23)$$

Using this and $q_1 \leq q_2$ we have

$$2(q_1 - q_2)\left(\frac{|g_1|^2}{q_1} - \frac{|g_2|^2}{q_2}\right) = 2\frac{(q_1 - q_2)}{q_1 q_2}\left(q_2|g_1|^2 - q_1|g_2|^2\right)$$

$$= 2\frac{(q_1 - q_2)}{q_1 q_2}\left((q_2 - q_1)|g_1|^2 - q_1(|g_2|^2 - |g_1|^2)\right)$$

$$\overset{(2.23)}{\leq} 0. \qquad (2.24)$$

The other possibility is

$$0 \leq (q_2 - q_1)|g_1|^2 \leq q_1 \big||g_1|^2 - |g_2|^2\big|. \tag{2.25}$$

In this case, we have (also using $q_1 \leq q_2$)

$$
\begin{aligned}
2(q_1 - q_2)\left(\frac{|g_1|^2}{q_1} - \frac{|g_2|^2}{q_2}\right) &= 2\frac{(q_1 - q_2)}{q_1 q_2}\Big((q_2 - q_1)|g_1|^2 - q_1(|g_2|^2 - |g_1|^2)\Big) \\
&\leq -2\frac{(q_1 - q_2)}{q_1 q_2} q_1(|g_2|^2 - |g_1|^2) \\
&\leq 2\frac{|q_1 - q_2|}{|q_2|}\big||g_2|^2 - |g_1|^2\big| \\
&\leq 2\frac{|q_1 - q_2|}{|q_1|}\big||g_2|^2 - |g_1|^2\big| \\
&\overset{(2.25)}{\leq} 2\frac{(|g_2|^2 - |g_1|^2)^2}{|g_1|^2}. \tag{2.26}
\end{aligned}
$$

Therefore, since $|g_1| \geq C_r > 0$ (by 2.19), we must have

$$2(q_1 - q_2)\left(\frac{|g_1|^2}{q_1} - \frac{|g_2|^2}{q_2}\right) \leq 2C_r^{-2}(|g_2|^2 - |g_1|^2)^2 \leq C(|q_1 - q_2|^2 + |h_1 - h_2|^2).$$

where $C > 0$ depends only on r. This establishes (2.22).

Returning to (2.21) and controlling the first term on the right hand side of (2.21) with (2.22), we conclude that

$$
\begin{aligned}
\widehat{\mathbb{E}}\left[(q_{1,t\wedge\tau} - q_{2,t\wedge\tau})^2\right] &\leq C\int_0^t \widehat{\mathbb{E}}\left[\mathbb{I}_{[0,\tau]}(s)(q_{1,s} - q_{2,s})^2\right] ds \\
&\quad + C\int_0^t \widehat{\mathbb{E}}\left[\mathbb{I}_{[0,\tau]}(s)|h_{1,s} - h_{2,s}|^2\right] ds + C|x_1 - x_2|, \\
&\leq C\int_0^t \widehat{\mathbb{E}}\left[(q_{1,s\wedge\tau} - q_{2,s\wedge\tau})^2\right] ds \\
&\quad + C\int_0^t \widehat{\mathbb{E}}\left[|h_{1,s\wedge\tau} - h_{2,s\wedge\tau}|^2\right] ds + C|x_1 - x_2|. \tag{2.27}
\end{aligned}
$$

By combining (2.20) and (2.27) and applying Gronwall's inequality, we conclude that

$$\widehat{\mathbb{E}}\left[|h_{1,t\wedge\tau} - h_{2,t\wedge\tau}|^2\right] + \widehat{\mathbb{E}}\left[(q_{1,t\wedge\tau} - q_{2,t\wedge\tau})^2\right] \leq C|x_1 - x_2|\left(1 + te^{Ct}\right), \quad t \geq 0. \tag{2.28}$$

Using (2.21) and (2.22) we also obtain

$$\widehat{\mathbb{E}}\left[\max_{t\in[0,T]}(q_{1,t\wedge\tau}-q_{2,t\wedge\tau})^2\right] \le C\int_0^T \widehat{\mathbb{E}}[(q_{1,s\wedge\tau}-q_{2,s\wedge\tau})^2]\,\mathrm{d}s$$

$$+C\int_0^T \widehat{\mathbb{E}}[|h_{1,s\wedge\tau}-h_{2,s\wedge\tau}|^2]\,\mathrm{d}s + C|x_1-x_2|$$

$$+\widehat{\mathbb{E}}\left[\max_{t\in[0,T]}V_t\right] \tag{2.29}$$

where V_t is the martingale

$$V_t = \int_0^{t\wedge\tau} 2(q_1-q_2)(g_1-g_2)\cdot\mathrm{d}\widehat{W}_s.$$

By the Burkholder–Davis–Gundy inequality (e.g. [30, Sec IV.4]) and (2.28), we have

$$\widehat{\mathbb{E}}\left[\max_{t\in[0,T]}V_t\right] \le C\left(\int_0^T \widehat{\mathbb{E}}[(q_{1,s\wedge\tau}-q_{2,s\wedge\tau})^2]\,\mathrm{d}s\right)^{1/2} \le C_T|x_1-x_2|^{1/2}.$$

This, together with (2.28) and (2.29), gives us

$$\widehat{\mathbb{E}}\left[\max_{t\in[0,T]}(q_{1,t\wedge\tau}-q_{2,t\wedge\tau})^2\right] \le C_T|x_1-x_2|^{1/2}.$$

Similar arguments for h_1-h_2 lead to

$$\widehat{\mathbb{E}}\left[\max_{t\in[0,T]}|h_{1,t\wedge\tau}-h_{2,t\wedge\tau}|^2\right] \le C_T|x_1-x_2|.$$

$\square$

Proof of Lemma 2.3 Suppose $\tau_r = 0$ holds with probability $\epsilon > 0$. Because of (2.6) we may choose m sufficiently large so that

$$\sum_{n=m}^{\infty}\max_{0\le t\le(T\wedge\widehat{\tau}^n)}|Y_t^{x_{n+1}}-Y_t^{x_n}| < r/4$$

holds with probability at least $1-\epsilon/2$. Therefore, with probability at least $\epsilon/2$ we have both $\tau_r = 0$ and

$$\liminf_{n\to\infty}|Y_{\tau_r^n}^{x_n}-Y_{\tau_r^n}^{x_m}| \le r/4. \tag{2.30}$$

Recall that $|Y_0^{x_m} - y_0| \le 25^{-m}$. Let m be larger, if necessary, so that $25^{-m} \le r/4$. This and (2.30) imply that

$$\liminf_{n \to \infty} |Y_{\tau_r^n}^{x_n} - y_0| \le \liminf_{n \to \infty} \left(|Y_{\tau_r^n}^{x_n} - Y_{\tau_r^n}^{x_m}| + |Y_{\tau_r^n}^{x_m} - y_0| \right) \le r/4 + 25^{-m} \le r/2$$

holds with probability at least $\epsilon/2$. However, this contradicts the fact that $Y_{\tau_r^n}^{x_n} \in \partial B_r(y_0)$ for all n. Hence, we must have $\tau_r > 0$ with probability one.   □

Proof of Lemma 2.4 The fact that $\overline{\tau}_{r/2} > 0$ with probability one follows from an argument very similar to the proof of Lemma 2.3. The fact that $\overline{\tau}_{r/2} < \tau_r$ will follow by showing that

$$\limsup_{t \nearrow \tau_r} |Y_t - y_0| \ge r \tag{2.31}$$

holds with probability one. First, suppose that $\tau_r^n < \tau_r$ and that

$$\tau_r^n = \inf_{k \ge n} \tau_r^k$$

Then by (2.6) we have

$$|Y_{\tau_r^n} - y_0| \ge |Y_{\tau_r^n}^{x_n} - y_0| - |Y_{\tau_r^n} - Y_{\tau^n}^{x_n}| = r - |Y_{\tau_r^n} - Y_{\tau_r^n}^{x_n}| = r - R(n).$$

where $R(n)$ is the series remainder

$$R(n) = \sum_{k=n}^{\infty} \max_{0 \le t \le \tau_r^n} |Y_t^{x_{k+1}} - Y_t^{x_k}|$$

which converges to zero, with probability one, as $n \to \infty$. So, with probability one, if there is an increasing sequence of such times $\tau_r^{n_j} \nearrow \tau_r$ as $j \to \infty$, we see that (2.31) must hold. On the other hand, suppose there is no such sequence. Then we must have $\tau_r^n \ge \tau_r$ for n sufficiently large. Hence $Y_t^{x_n}$ must converge to Y_t uniformly on the closed interval $[0, \tau_r]$. Suppose $\tau_r^n \ge \tau_r$ and $\tau_r^n = \sup_{k \ge n} \tau_r^k$. Then for all $k \ge n$, we have

$$|Y_{\tau_r^k}^{x_n} - y_0| \ge |Y_{\tau_r^k}^{x_k} - y_0| - |Y_{\tau_r^k}^{x_n} - Y_{\tau_r^k}^{x_k}|$$
$$= r - |Y_{\tau_r^k}^{x_n} - Y_{\tau_r^k}^{x_k}| \ge r - M(n).$$

Therefore, since $Y_t^{x_n}$ is continuous on $[0, \tau_r^n]$ and since $\tau_r = \liminf_{k \ge 0} \tau_r^k$, we have

$$|Y_{\tau_r}^{x_n} - y_0| \ge r - M(n).$$

Since $Y_{\tau_r}^{x_n} \to Y_{\tau_r}$ in this case and Y_t is continuous on $[0, \tau_r]$, then with probability one, this case also implies that (2.31) holds. Having established that $0 < \overline{\tau}_{r/2} < \tau_r$ we conclude that $Y_t^{x_n} \to Y_t$ uniformly on $[0, \overline{\tau}_{r/2}]$. Since each $Y_t^{x_n}$ is $\widehat{\mathcal{F}}_t$-adapted, so is the limit Y_t. In particular, $\overline{\tau}_{r/2}$ is a stopping time.   □

Remark 2.5 Let us point out that if $y_0 \in \partial A$ and $T > 0$ is sufficiently small, the equation

$$\overline{Y}(t) = y_0 + \int_0^t K(\overline{Y}(s)) \, ds, \quad t \in [0, T]. \tag{2.32}$$

has a unique solution satisfying $\overline{Y}(t) \in \Theta$ for all $t \in (0, T]$. Indeed, let $z(t)$ solve the ODE

$$z'(t) = 2a(z(t))\nabla q(z(t)) + q(z(t))b(z(t))$$

for $t \in [0, T]$, with $z(0) = y_0$. For sufficiently small T, $z(s) \in \Theta$ for $t \in (0, T]$. Hence $q(z(s)) > 0$ for $t \in (0, T]$ and the function $F(t) = \int_0^t q(z(s)) \, ds$ is invertible. Now, it is easy to check that the function $\overline{Y}(t) = z(F^{-1}(t))$ is continuous on $[0, T]$ and satisfies (2.32). Moreover, $\overline{Y}(t) \in \Theta$ for all $t \in (0, T]$. In fact,

$$\overline{Y}(t) \sim y_0 + 2\sqrt{t} \, \frac{a(y_0)\nabla q(y_0)}{\langle \nabla q(y_0), a(y_0)\nabla q(y_0)\rangle^{1/2}}$$

for small t.

We state and prove two properties of the transition path process, which will be used later.

Proposition 2.6 *Let F be a bounded and continuous functional on $C([0, \infty))$. Define*

$$g(x) = \widehat{\mathbb{E}}[F(Y) \mid Y_0 = x]$$

where Y_t satisfies (1.14). *Then $g \in C(\overline{\Theta})$.*

Proof Suppose that $\{x_n\}_{n=1}^\infty \subset \overline{\Theta}$ and that $x_n \to x \in \overline{\Theta}$ as $n \to \infty$. We claim that there must be a subsequence $\{x_{n_j}\}_{j=1}^\infty$ such that, $\mathbb{Q}$-almost surely,

$$\lim_{j \to \infty} F(Y^j) = F(Y), \tag{2.33}$$

where Y_t^j satisfies (1.14) with $Y_0^j = x_{n_j}$, and Y_t satisfies (1.14) with $Y_0 = x$. Since F is bounded and continuous on $C([0, \infty))$, the dominated convergence theorem then implies that

$$\lim_{j \to \infty} g(x_{n_j}) = \lim_{j \to \infty} \widehat{\mathbb{E}}[F(Y) \mid Y_0 = x_{n_j}] = \widehat{\mathbb{E}}[F(Y) \mid Y_0 = x] = g(x).$$

Since the limit is independent of the subsequence, this implies that $g(x)$ is continuous.

To establish (2.33), we must show that $Y_t^j \to Y_t$ uniformly on compact subsets of $[0, \infty)$. This follows from Corollary 2.2, as in the proof of Theorem 1.1. $\qquad \square$

Proposition 2.7 *For any $R > 0$, there is a function $h_R : [0, +\infty) \to [0, 1]$ such that $\int_0^\infty h_R(t) \, dt < +\infty$ and*

$$\sup_{\substack{x \in \Theta \\ |x| \leq R}} \mathbb{Q}(Y_t \in \Theta \mid Y_0 = x) \leq h_R(t).$$

holds for all $t \geq 0$.

Proof If $x \in \Theta$, then by the Doob h-transform, we know that

$$
\begin{aligned}
\mathbb{Q}(Y_t \in \Theta \mid Y_0 = x) &= \frac{\mathbb{P}(X_s \in \Theta \; \forall s \in [0, t], \; \tau_B < \tau_A \mid X_0 = x)}{\mathbb{P}(\tau_B < \tau_A \mid X_0 = x)} \\
&\leq \frac{\mathbb{P}(X_s \in \Theta \; \forall s \in [0, t] \mid X_0 = x) \wedge \mathbb{P}(\tau_B < \tau_A \mid X_0 = x)}{\mathbb{P}(\tau_B < \tau_A \mid X_0 = x)} \\
&= \frac{\mathbb{P}(\tau_{AB} > t \mid X_0 = x) \wedge q(x)}{q(x)},
\end{aligned}
$$

where τ_{AB} is the first hitting time of X to $\overline{A} \cup \overline{B}$. Let $\alpha > 1$ be as in assumption (1.4). Since $\overline{A} \cup \overline{B}$ has non-empty interior and since $\sigma \sigma^T$ is uniformly positive definite, assumption (1.4) implies that for each $R > 0$ there is C_R such that

$$\sup_{|x| \leq R} \mathbb{E}[\tau_{AB}^\alpha \mid X_0 = x] < C_R.$$

From this and Chebychev's inequality, it follows that

$$\sup_{|x| \leq R} \mathbb{P}(\tau_{AB} > t \mid X_0 = x) \leq t^{-\alpha} \sup_{|x| \leq R} \mathbb{E}[\tau_{AB}^\alpha \mid X_0 = x] \leq C_R \, t^{-\alpha} \quad (2.34)$$

holds for all $t > 0$. So, for any $\epsilon > 0$,

$$\mathbb{Q}(Y_t \in \Theta \mid Y_0 = x) \leq \frac{C_R \, t^{-\alpha} \wedge \epsilon}{\epsilon} \quad (2.35)$$

holds for all $t > 0$ and $x \in \{x \in \Theta \mid |x| \leq R, \; q(x) \geq \epsilon\}$.

The bound (2.35) does not include points near ∂A, where $q(x) < \epsilon$. Fix $\epsilon \in (0, 1)$ and define the set $S = \{x \in \Theta \mid q(x) < \epsilon\} \cup \overline{A}$. If ϵ is small enough, this set is bounded and we may assume $|x| < R$ for all $x \in S$. Suppose $Y_0 = x$ with $x \in S \cap \overline{\Theta}$. Let $q_t = q(Y_t)$, which satisfies

$$q_t = q_0 + \int_0^t \frac{|g(Y_s)|^2}{q_s} \, ds + \int_0^t g(Y_s) \, d\widehat{W}_s$$

where $g(y) = \sqrt{2}(\nabla q(y))^T \sigma(y)$. By (1.9) we know that if $\epsilon > 0$ is small enough, there is a constant $C_\epsilon > 0$ such that $|g(y)|^2 \geq C_\epsilon$ for all $y \in \overline{S} \cap \overline{\Theta}$. Therefore, if

$Y_t \in \overline{S} \cap \overline{\Theta}$ for all $t \in [0, T]$, we must have $q_t \leq \epsilon$ for all $t \in [0, T]$ and

$$q_t \geq \int_0^t \frac{C_\epsilon}{q_s} \, ds + \int_0^t g(Y_s) \, d\widehat{W}_s \geq t\epsilon^{-1} C_\epsilon + \int_0^t g(Y_s) \, d\widehat{W}_s$$

for all $t \in [0, T]$. This happens only if the martingale $M_t = \int_0^t g(Y_s) \, d\widehat{W}_s$ satisfies

$$M_t \leq \epsilon - t\epsilon^{-1} C_\epsilon, \quad t \in [0, T].$$

To control the probability of this event, for any $\gamma > 0, \beta > 0, T > 0$, Chebychev's inequality implies

$$\mathbb{Q}(M_T \leq -\gamma T) \leq e^{-\beta \gamma T} \widehat{\mathbb{E}}[e^{-\beta M_T}] \leq e^{-\beta \gamma T} \widehat{\mathbb{E}}\left[\exp\left(\frac{\beta^2}{2} \int_0^T |g|^2 \, ds \right) \right]$$

$$\leq e^{-\beta \gamma T + \frac{\beta^2}{2} \|g\|_\infty^2 T}.$$

By choosing $\beta = \gamma / \|g\|_\infty^2$ we have $\mathbb{Q}(M_T \leq -\gamma T) \leq e^{-\gamma^2 C_1 T}$. Hence there is a constant $C_2 > 0$ such that

$$\mathbb{Q}\left(Y_t \in \overline{S} \cap \overline{\Theta}, \quad \forall \, t \in [0, T] \mid Y_0 = x \right) \leq e^{-\epsilon^2 C_2 T} \tag{2.36}$$

holds for all $T > 1$ and $x \in \overline{S} \cap \overline{\Theta}$.

Now we combine (2.35) and (2.36). Let $\tau_S = \inf\{t > 0 \mid Y_t \in \partial S\}$. By (2.36) we have $\mathbb{Q}(\tau_S > t/2 \mid Y_0 = x) \leq e^{-C_3 t}$ holds for all $x \in \overline{S} \cap \overline{\Theta}$. Therefore, since τ_S is a stopping time, we conclude that

$$\mathbb{Q}(Y_t \in \Theta \mid Y_0 \in x) \leq \mathbb{Q}(Y_t \in \Theta, \tau_S < t/2 \mid Y_0 \in x) + e^{-C_3 t}$$

$$\leq \sup_{y \in \partial S} \mathbb{Q}\left(Y_{t/2} \in \Theta \mid Y_0 \in y \right) + e^{-C_3 t}$$

$$\leq \frac{Ct^{-\alpha} \wedge \epsilon}{\epsilon} + e^{-C_3 t}.$$

for all $x \in \overline{S} \cap \overline{\Theta}$. Since the last expression is an integrable function of t, this completes the proof. $\square$

Proof of Theorem 1.2 Since $\tau_{A,n}^+$ is a stopping time, it suffices to prove the result for $n = 0$. Fix $\epsilon > 0$ and let $S \supset \overline{A}$ be the open set

$$S = \{x \in \Theta \mid q(x) < \epsilon\} \cup \overline{A}.$$

For $\epsilon > 0$ small, this is a bounded set that separates A and B. The boundary ∂S is an isosurface for q: $q(x) = \epsilon$ for $x \in \partial S$. As $\epsilon \to 0$, S shrinks to A, and the Hausdorff distance $d_{\mathcal{H}}(\partial S, \partial A)$ is $\mathcal{O}(\epsilon)$ (because of (1.9)).
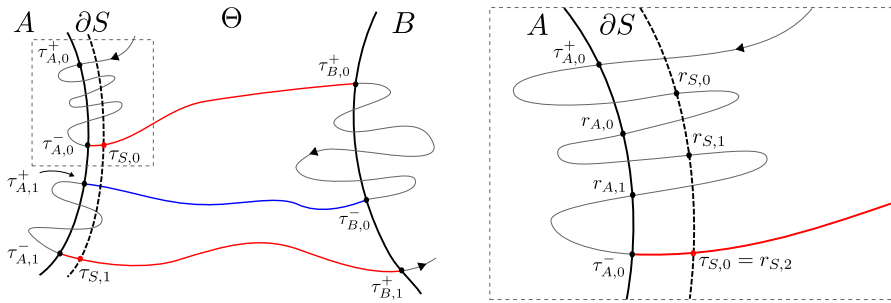
Fig. 2 *Left panel* The set S and random times $\tau_{S,j}$. *Right panel* Zoom-in of the *boxed* region together with stopping times $r_{S,k}$ and $r_{A,k}$

Recalling that $\tau_{A,0}^+ = \inf\{t \geq 0 \mid X_t \in \overline{A}\}$, we define

$$r_{S,0} = \inf\{t > \tau_{A,0}^+ \mid X_t \in \partial S\}.$$

which is a stopping time with respect to $\mathcal{F}_t$. Then for $k \geq 0$, we define inductively the stopping times (see Fig. 2)

$$r_{A,k} = \inf\left\{t > r_{S,k} \mid X_t \in \overline{A}\right\},$$
$$r_{B,k} = \inf\left\{t > r_{S,k} \mid X_t \in \overline{B}\right\},$$
$$r_{S,k+1} = \inf\left\{t > r_{A,k} \mid X_t \in \partial S\right\}.$$

Observe that $r_{S,k} < r_{A,k} < r_{S,k+1}$, although it is possible that $r_{B,k} = r_{B,k+1}$. Let $r_{AB,k} = r_{A,k} \wedge r_{B,k}$, which is finite with probability one. We also define the random time

$$\tau_{S,j} = \inf\left\{t > \tau_{A,j}^- \mid X_t \in \partial S\right\}.$$

Although $\tau_{S,j}$ is not a stopping time with respect to $\mathcal{F}_t$, the relation

$$\left\{r_{S,k} \mid k \geq 0, \ r_{B,k} < r_{A,k}\right\} = \{\tau_{S,j}\}_{j=0}^\infty \tag{2.37}$$

holds $\mathbb{P}$-almost surely.

Now, let

$$Y_t^0 = X_{(t+\tau_{A,0}^-)\wedge\tau_{B,0}^+}, \qquad t \geq 0,$$

and let $h_0 = \tau_{S,0} - \tau_{A,0}^-$. Since F is bounded and continuous, and since $h_0 \to 0$ ($\mathbb{P}$ almost surely) as $\epsilon \to 0$, we have

$$\mathbb{E}[F(X_{\cdot+\tau_{A,0}^-})] = \mathbb{E}[F(Y_\cdot^0)] = \lim_{\epsilon \to 0} \mathbb{E}[F(Y_{\cdot+h_0}^0)]. \tag{2.38}$$

We will show that

$$\lim_{\epsilon \to 0} \mathbb{E}[F(Y^0_{\cdot +h_0})] = \mathbb{E}[g(X_{\tau^-_{A,0}})]$$

where $g(x) = \widehat{\mathbb{E}}[F(Y_\cdot) \mid Y_0 = x]$.

Let M be the unique (random) integer such that

$$\tau_{S,0} = r_{S,M}.$$

Equivalently, $M = \min\{k \geq 0 \mid r_{B,k} < r_{A,k}\}$. Since $r_{B,k} > r_{A,k}$ for all $k < M$, we have

$$F(Y^0_{\cdot +h_0}) = \sum_{k=0}^{M} F(X_{\cdot +r_{S,k}}) \mathbb{I}_{r_{B,k} < r_{A,k}} = \sum_{k=0}^{\infty} F(X_{\cdot +r_{S,k}}) \mathbb{I}_{r_{B,k} < r_{A,k}} \mathbb{I}_{k \leq M}. \qquad (2.39)$$

Observe that the event $\{k \leq M\}$ coincides with the event that $r_{B,j} > r_{A,j}$ for all $j < k$, so the event $\{k \leq M\}$ is measurable with respect to $\mathcal{F}_{rS,k}$. Therefore, we have

$$\mathbb{E}[F(Y^0_{\cdot +h_0})] = \sum_{k=0}^{\infty} \mathbb{E}\left[F(X_{\cdot +r_{S,k}}) \mathbb{I}_{r_{B,k} < r_{A,k}} \mathbb{I}_{k \leq M}\right]$$

$$= \sum_{k=0}^{\infty} \mathbb{E}\left[\mathbb{E}[F(X_{\cdot +r_{S,k}}) \mathbb{I}_{r_{B,k} < r_{A,k}} \mathbb{I}_{k \leq M} \mid \mathcal{F}_{rS,k}]\right]$$

$$= \sum_{k=0}^{\infty} \mathbb{E}\left[\mathbb{I}_{k \leq M} \mathbb{E}[F(X_{\cdot +r_{S,k}}) \mathbb{I}_{r_{B,k} < r_{A,k}} \mid \mathcal{F}_{rS,k}]\right]$$

$$= \sum_{k=0}^{\infty} \mathbb{E}\left[\mathbb{I}_{k \leq M} \, f(X_{r_{S,k}})\right],$$

where

$$f(x) = \mathbb{E}[F(X_\cdot) \mathbb{I}_{\tau_B < \tau_A} \mid X_0 = x] = q(x)\widehat{\mathbb{E}}[F(Y_\cdot) \mid Y_0 = x].$$

The last equality follows from the Doob h-transform (since $x \in \partial S \subset \Theta$ here). Since $q(x) = \epsilon$ for all $x \in \partial S$, this means

$$\mathbb{E}[F(Y^0_{\cdot +h_0})] = \epsilon \, \mathbb{E}\left[\sum_{k=0}^{M} g(X_{r_{S,k}})\right] \qquad (2.40)$$

where $g(x) = \widehat{\mathbb{E}}[F(Y_\cdot) \mid Y_0 = x]$. Note that the random integer M depends on ϵ.

Let A_j denote the event $\{j < M\}$, which occurs if and only if $r_{A,k} < r_{B,k}$ for all $k \in \{0, 1, \ldots, j\}$. Since $q(x) = \epsilon$ for all $x \in \partial S$, the event A_j is independent of $X_{r_{S,j}} \in \partial S$. Moreover, $P(A_j) = (1 - \epsilon)^{j+1}$, since

$$\mathbb{P}(A_j) = \mathbb{E}\left[\prod_{k=0}^{j} \mathbb{I}_{r_{A,k} < r_{B,k}}\right]$$

$$= \mathbb{E}\left[\prod_{k=0}^{j-1} \mathbb{I}_{r_{A,k} < r_{B,k}} \, \mathbb{E}[\mathbb{I}_{r_{A,j} < r_{B,j}} \mid \mathcal{F}_{r_{S,j}}]\right] = (1 - \epsilon)\mathbb{P}(A_{j-1}).$$

Similarly, $\mathbb{P}(M = j) = \epsilon(1 - \epsilon)^j$. Now we evaluate (2.40):

$$\mathbb{E}[F(Y^0_{\cdot + h_0})] = \epsilon \, \mathbb{E}[g(X_{r_{S,0}})] + \epsilon \, \mathbb{E}\left[\sum_{k=1}^{M} g(X_{r_{S,k}})\right]$$

$$= \epsilon \, \mathbb{E}[g(X_{r_{S,0}})] + \epsilon \, \mathbb{E}\left[\sum_{j=0}^{\infty} \mathbb{I}_{A_j} \, g(X_{r_{S,j+1}})\right]$$

$$= \epsilon \, \mathbb{E}[g(X_{r_{S,0}})] + \epsilon \sum_{j=0}^{\infty} \mathbb{E}\left[\mathbb{I}_{A_j} \, g(X_{r_{S,j+1}})\right]$$

$$= \epsilon \, \mathbb{E}[g(X_{r_{S,0}})] + \epsilon \sum_{j=0}^{\infty} \mathbb{P}(A_j) \, \mathbb{E}\left[g(X_{r_{S,j+1}})\right]$$

$$= \epsilon \, \mathbb{E}[g(X_{r_{S,0}})] + \epsilon \sum_{j=0}^{\infty} (1 - \epsilon)^{j+1} \mathbb{E}\left[g(X_{r_{S,j+1}})\right]$$

$$= \sum_{j=0}^{\infty} \epsilon(1 - \epsilon)^j \, \mathbb{E}\left[g(X_{r_{S,j}})\right]$$

$$= \sum_{j=0}^{\infty} \mathbb{P}(M = j) \mathbb{E}\left[g(X_{r_{S,j}})\right] = \mathbb{E}\left[g(X_{\tau_{S,0}})\right].$$

Now let $\epsilon \to 0$. Since $g(x)$ is bounded and is continuous up to ∂A by Proposition 2.6, we have (by the dominated convergence theorem)

$$\lim_{\epsilon \to 0} \mathbb{E}\left[g(X_{\tau_{S,0}})\right] = \mathbb{E}\left[\lim_{\epsilon \to 0} g(X_{\tau_{S,0}})\right] = \mathbb{E}\left[g(X_{\tau_{A,0}^-})\right]. \qquad (2.41)$$

$\square$

3 Reactive exit and entrance distributions

Proof of Lemma 1.3 The equality (1.22) is equivalent to

$$\int_{\partial \Theta} \rho(x)\widehat{n}(x) \cdot a(x)\nabla q(x) \, d\sigma_\Theta(x) = 0.$$

Using (1.19), it is then equivalent to

$$\langle \rho, Lq \rangle = \langle L^*\rho, q \rangle = 0,$$

which is obvious. □

Before proving Proposition 1.5, we will need to establish some properties of the entrance and exit distributions and of the harmonic measure associated with the generator L. These results will also be used later in the paper. First, using integration by parts, we have

Lemma 3.1 *Let $D \subset \mathbb{R}^d$ be open with smooth boundary. Let $\phi, \psi \in C^2(D) \cap C^1(\overline{D})$ and bounded. Then*

$$\int_D \rho(x)\big(\phi(x)L\psi(x) - \psi(x)\widetilde{L}\phi(x)\big)\, \mathrm{d}x = \int_{\partial D} \rho(x)b \cdot \widehat{n}(x)\phi(x)\psi(x)\, \mathrm{d}\sigma_D(x)$$

$$+ \int_{\partial D} \rho(x)\phi(x)\widehat{n}(x) \cdot a\nabla\psi(x) - \psi(x)\widehat{n}(x) \cdot \mathrm{div}(a(x)\rho(x)\phi(x))\, \mathrm{d}\sigma_D(x), \quad (3.1)$$

where $\widehat{n}(x)$ is the exterior normal vector at $x \in \partial D$.

Let us recall some tools from potential theory (see for example the books [28, 32] and also [7,8] where potential theory was applied to analyze diffusion processes with metastability). The harmonic measure $H_D(x, \mathrm{d}y)$ is given by the Poisson kernel corresponding to the boundary value problem

$$\begin{cases} Lu(x) = 0, & x \in D, \\ u(x) = f(x), & x \in \partial D. \end{cases} \quad (3.2)$$

Therefore, for $f \in C(\partial D)$,

$$u(x) = \int_{\partial D} H_D(x, \mathrm{d}y)f(y), \quad (3.3)$$

is the unique solution to (3.2). Similarly, the harmonic measure $\widetilde{H}_D(x, \mathrm{d}y)$ corresponds to the generator $\widetilde{L}$ (recall (1.28)). For the boundary value problem

$$\begin{cases} \widetilde{L}\widetilde{u}(x) = 0, & x \in D, \\ \widetilde{u}(x) = f(x), & x \in \partial D, \end{cases} \quad (3.4)$$

the solution is given by

$$\widetilde{u}(x) = \int_{\partial D} \widetilde{H}_D(x, \mathrm{d}y)f(y). \quad (3.5)$$

The harmonic measures have a probabilistic interpretation: $H_D(x, \mathrm{d}y)$ (resp. $\widetilde{H}_D(x, \mathrm{d}y)$) gives the probability that the process associated with the generator L (resp. $\widetilde{L}$) first strikes the boundary ∂D at $\mathrm{d}y$ after starting at x. In particular,

$$q(x) = H_D(x, \partial B) \quad \text{and} \quad \widetilde{q}(x) = \widetilde{H}_D(x, \partial A).$$

We also define the harmonic measures for the conditioned processes as

$$H_{\Theta}^q(x, dy) = \frac{q(y)}{q(x)} H_{\Theta}(x, dy). \tag{3.6}$$

For $x \in \Theta$ this is a measure on ∂B. For $x \in \partial A$ where $q(x) = 0$, we may define $H_{\Theta}^q(x, dy)$ through a limit:

$$H_{\Theta}^q(x, dy) = \lim_{\substack{x' \in \Theta \\ x' \to x}} \frac{q(y)}{q(x)} H_{\Theta}(x, dy) = \frac{\widehat{n}(x) \cdot a(x) \nabla_x H_{\Theta}(x, dy)}{\widehat{n}(x) \cdot a(x) \nabla_x q(x)}, \quad x \in \partial A. \tag{3.7}$$

Recall that $q(y) = 1$ for $y \in \partial B$.

Recall the reactive exit and entrance measures η_A^-, η_A^+, η_B^- and η_B^+. They are connected by harmonic measures as follows:

Proposition 3.2

$$\int_{\partial A} \eta_A^-(dx) H_{\Theta}^q(x, dy) = \eta_B^+(dy). \tag{3.8}$$

$$\int_{\partial A} \eta_A^+(dx) H_{\overline{B}^c}(x, dy) = \eta_B^+(dy). \tag{3.9}$$

$$\int_{\partial B} \eta_B^+(dx) H_{\overline{A}^c}(x, dy) = \eta_A^+(dy). \tag{3.10}$$

Proof We prove (3.8) first. If $f \in C(\partial B)$, let $u_f(x)$ solve $Lu = 0$ in Θ with

$$u = \begin{cases} f(x), & x \in \partial B, \\ 0, & x \in \partial A. \end{cases} \tag{3.11}$$

Hence $u(x)\widetilde{q}(x) = 0$ on $\partial \Theta$. By applying (3.1) with $\phi(x) = \widetilde{q}(x)$ and $\psi(x) = u_f(x)$, we obtain

$$\int_{\partial A} \rho(x)\widehat{n}(x) \cdot a(x) \nabla u_f(x) \, d\sigma_A(x) = \int_{\partial B} f(x)\widehat{n}(x) \cdot \text{div}(a(x)\rho(x)\widetilde{q}(x)) \, d\sigma_B(x)$$

$$= \int_{\partial B} f(x)\rho(x)\widehat{n}(x) \cdot a(x) \nabla \widetilde{q}(x) \, d\sigma_B(x)$$

$$= -\int_{\partial B} f(x)\eta_B^+(dx). \tag{3.12}$$

From (3.7) and (1.23), we see that for all $x \in \partial A$,

$$\int_{\partial A} \eta_A^-(dx) H_\Theta^q(x, dy) = -\int_{\partial A} \rho(x) \widehat{n}(x) \cdot a(x) \nabla_x H_\Theta(x, dy) \, d\sigma_A(x).$$

Hence for any $f \in C(\partial B)$, we have

$$\int_{\partial B} \left(\int_{\partial A} \eta_A^-(dx) H_\Theta^q(x, dy) \right) f(y)$$

$$= -\int_{\partial B} \int_{\partial A} \rho(x) \widehat{n}(x) \cdot a(x) \nabla_x \left(f(y) H_\Theta(x, dy) \right) d\sigma_A(x)$$

$$= -\int_{\partial A} \rho(x) \widehat{n}(x) \cdot a(x) \nabla_x \left(\int_{\partial B} H_\Theta(x, dy) f(y) \right) d\sigma_A(x)$$

$$= -\int_{\partial A} \rho(x) \widehat{n}(x) \cdot a(x) \nabla_x u_f(x) \, dx.$$

Combining this with (3.12), we conclude that

$$\int_{\partial B} \left(\int_{\partial A} \eta_A^-(dx) H_\Theta^q(x, dy) \right) f(y) = \int_{\partial B} f(x) \eta_B^+(dx), \quad \forall f \in C(\partial B),$$

which proves (3.8).

To prove (3.9), let ψ solve $L\psi = 0$ for $x \in \overline{B}^c$ with $\psi = f$ on ∂B. Then by (3.1) with $\phi = 1 - \widetilde{q}$, we have

$$\int_{\partial A} \eta_A^+(dx) \psi(x) = \int_{\partial A} \rho(x) \widehat{n}(x) \cdot a(x) \nabla \widetilde{q}(x) \psi(x) \, d\sigma_A(x)$$

$$= -\int_{\partial A} \rho(x) \widehat{n}(x) \cdot a(x) \nabla (1 - \widetilde{q}(x)) \psi(x) \, d\sigma_A(x)$$

$$= -\int_{\partial A} \psi(x) \widehat{n}(x) \cdot \operatorname{div}(a\rho(1 - \widetilde{q})) \, d\sigma_A(x)$$

$$\left(\text{since } 1 - \widetilde{q} = 0 \text{ on } \partial A \right)$$

$$= \int_{\partial B} f \widehat{n} \cdot \operatorname{div}(a\rho(1 - \widetilde{q})) \, d\sigma_B(x) - \int_{\partial B} f \rho b \cdot \widehat{n} \, d\sigma_B(x)$$

$$- \int_{\partial B} \rho \widehat{n} \cdot a \nabla \psi \, d\sigma_B(x).$$

Applying (3.1) with the function $\phi \equiv 1$, we also find that

$$0 = -\int_{\partial B} f\widehat{n} \cdot \text{div}(a\rho) \, d\sigma_B(x) + \int_{\partial B} f\rho b \cdot \widehat{n} \, d\sigma_B(x) + \int_{\partial B} \rho \widehat{n} \cdot a\nabla\psi \, d\sigma_B(x).$$

Therefore, since $1 - \widetilde{q} = 1$ on ∂B, we conclude that

$$\int_{\partial A} \eta_A^+(dx)\psi(x) = \int_{\partial B} f\widehat{n} \cdot \text{div}(a\rho(1-\widetilde{q})) \, d\sigma_B(x) - \int_{\partial B} f\widehat{n}(x) \cdot \text{div}(a\rho) \, d\sigma_B(x)$$

$$= \int_{\partial B} f\rho\widehat{n} \cdot a\nabla(1-\widetilde{q}) \, d\sigma_B(x)$$

$$= -\int_{\partial B} f\rho\widehat{n} \cdot a\nabla\widetilde{q} \, d\sigma_B(x) = \int_{\partial A} f\eta_B^+(dx).$$

We arrive at (3.9) noting that

$$\psi(x) = \int_{\partial B} H_{\overline{B}^c}(x, dy) f(y).$$

We omit the proof of (3.10) which is analogous to that of (3.9) by switching the role of A and B. $\qquad\square$

By combining (3.9) and (3.10) we immediately obtain the following:

Corollary 3.3 *Let $P_B(x, dy)$ be the probability transition kernel*

$$P_B(x, dy) = \int_{\partial A} H_{\overline{A}^c}(x, dz) H_{\overline{B}^c}(z, dy), \quad x, y \in \partial B$$

on ∂B, and let $P_A(x, dy)$ be the probability transition kernel

$$P_A(x, dy) = \int_{\partial B} H_{\overline{B}^c}(x, dz) H_{\overline{A}^c}(z, dy), \quad x, y \in \partial A$$

on ∂A. Then

$$\int_{x \in \partial B} \eta_B^+(dx) P_B(x, dy) = \eta_B^+(dy).$$

and

$$\int_{x \in \partial A} \eta_A^+(dx) P_A(x, dy) = \eta_A^-(dy).$$

That is, η_B^+ and η_A^+ are invariant under P_B and P_A, respectively.

We are ready to return to the proof of Proposition 1.5.

Proof of Proposition 1.5 We first verify that η_B^+ is a probability measure. Taking $\psi = q$ and $\phi = \widetilde{q}$ in (3.1), we obtain using the boundary conditions of q and $\widetilde{q}$ on ∂A and ∂B,

$$\eta_A^-(\partial A) = \frac{1}{\nu} \int_{\partial A} \rho \widehat{n} \cdot a \nabla q \, d\sigma_A = \frac{1}{\nu} \int_{\partial B} \widehat{n} \cdot \text{div}(a \rho \widetilde{q}) \, d\sigma_B$$

$$= \frac{1}{\nu} \int_{\partial B} \widehat{n} \cdot a \rho \nabla \widetilde{q} \, d\sigma_B = \eta_B^+(\partial B).$$

This shows that $\eta_B^+(\partial B) = 1$ and ν is the correct normalization constant.

Let g be a positive continuous function on ∂B. Define for $x \notin \overline{B}$,

$$u(x) = \mathbb{E}\left[g(X_{\tau_B}) \mid X_0 = x\right]. \tag{3.13}$$

Hence u satisfies the equation

$$\begin{cases} Lu(x) = 0, & x \in \overline{B}^c; \\ u(x) = g(x), & x \in \partial B. \end{cases} \tag{3.14}$$

Let $H_{\overline{B}^c}(x, dy)$ be the harmonic measure (the measure of the first hitting point on $\overline{B}$ for the process starting at x). We have

$$u(x) = \int_{\partial B} H_{\overline{B}^c}(x, dy) g(y). \tag{3.15}$$

By the maximum principle, $u > 0$ in $\overline{B}^c$. By the Harnack inequality for non-divergence form elliptic operators [18, Corollary 9.25] and the compactness of ∂A, we have

$$\sup_{x \in \partial A} u(x) \leq C \inf_{x \in \partial A} u(x), \tag{3.16}$$

where the constant $C > 0$ only depends on the elliptic constants of $a(x)$ and on the maximum of $|b|$ over some compact set A' satisfying $A \subset A' \subset \overline{B}^c$. In particular, C is independent of g. Therefore, we obtain for any $x, x' \in \partial A$, $y \in \partial B$

$$0 < C^{-1} \leq \frac{H_{\overline{B}^c}(x, dy)}{H_{\overline{B}^c}(x', dy)} \leq C < \infty. \tag{3.17}$$

If we define

$$\nu_B(dy) = \inf_{x \in \partial A} H_{\overline{B}^c}(x, dy), \tag{3.18}$$

then $\nu_B(E) > 0$ is absolutely continuous with respect to $\sigma_B(dy)$ on ∂B, and

$$H_{\overline{B}^c}(x, dy) \geq C^{-1}\nu_B(dy) \tag{3.19}$$

for any $x \in \partial A$.

Consider the Markov chain given by $\{X_{\tau_{B,k}^+}\}_{k=0}^{\infty}$ on ∂B. Let P_B denote its transition kernel, given by

$$P_B(y, dy') = \int_{\partial A} H_{\overline{A}^c}(y, dx) H_{\overline{B}^c}(x, dy'). \tag{3.20}$$

By (3.19), P_B satisfies Doeblin's minorization condition:

$$P_B(y, dy') \geq C^{-1} \int_{\partial A} H_{\overline{A}^c}(y, dx)\nu_B(dy') = C^{-1}\nu_B(dy'). \tag{3.21}$$

Therefore, P_B has a unique invariant measure [3, Theorem 6.1]. By Corollary 3.3, this invariant measure is given by η_B^+. Hence, as $N \to \infty$, $\int_{\partial B} f(x) \, d\mu_{B,N}^+(x)$ converges exponentially fast to $\int_{\partial B} f(x) \, d\eta_B^+(x)$ (see e.g. [26, Theorem 17.1.7]). The rate of the convergence depends on the sets A and B. $\square$

Proof of Theorem 1.7 Consider the family of processes

$$X_t^{A,n} = X_{(t+\tau_{A,n}^+)\wedge\tau_{B,n}^+}.$$

Observe that the nth reactive trajectory $t \mapsto Y_t^n$ is a subset of the path $t \mapsto X_t^{A,n}$; specifically, $Y_t^n = X_{t+\tau_{A,n}^- - \tau_{A,n}^+}^{A,n}$ for all $t \geq 0$. The random sequence of points

$$y_n = X_0^{A,n} = X_{\tau_{A,n}^+} \in \partial A, \quad n = 0, 1, 2, \ldots$$

corresponds to a Markov chain on the state space ∂A with transition kernel

$$P_A(x, dy) = \mathbb{P}(y_{n+1} \in dy \mid y_n = x) = \int_{\partial B} H_{\overline{B}^c}(x, dz) H_{\overline{A}^c}(z, dy).$$

As shown in the proof of Proposition 1.5 (reversing the role of B and A), this chain satisfies a Doeblin minorizing condition

$$P_A(x, dy) \geq C^{-1}\nu_A(dy) = C^{-1} \inf_{x\in\partial B} H_{\overline{A}^c}(x, dy) > 0, \tag{3.22}$$

and the chain has a unique invariant probability distribution η_A^+ supported on ∂A:

$$\int_{\partial A} \eta_A^+(dx) P_A(x, dy) = \eta_A^+(dy).$$

The sequence of processes $t \mapsto X_t^{A,n}$ corresponds to a homogeneous Markov chain on the metric space $\mathcal{X} = C([0, \infty))$. The transition probability K for this chain may be expressed as follows. If $X \in C([0, \infty))$ is such that $\tau_B^X = \inf\{t \geq 0 \mid X_t \in \partial B\}$ is finite, then for any set $E \in \mathcal{B}$,

$$K(X, E) = \mathbb{P}(X^{A,n+1} \in E \mid X^{A,n} = X) = \int_{\partial A} H_{\overline{A}^c}(X_{\tau_B^X}, dy)\mathcal{P}_y(E), \qquad (3.23)$$

where $\mathcal{P}_x$ denotes the law on $(\mathcal{X}, \mathcal{B})$ of the process $t \mapsto Z_{t \wedge \tau_B}$ where

$$dZ_t = b(Z_t)\, dt + \sqrt{2}\, \sigma(Z_t)\, dW_t, \quad Z_0 = x$$

and τ_B is the first hitting time of Z_t to $\overline{B}$. If $X \in C([0, \infty))$ never hits the set $\overline{B}$, then we define

$$K(X, E) = \int_{\partial A} \eta_A^+(dy)\mathcal{P}_y(E), \quad E \in \mathcal{B}. \qquad (3.24)$$

This chain on $\mathcal{X}$ has a unique invariant distribution

$$\overline{\mathcal{P}}(U) = \int_{\partial A} \eta_A^+(dy)\mathcal{P}_y(U), \quad \forall\, U \in \mathcal{B},$$

supported on the set of paths which originate in ∂A and are constant after hitting ∂B. The uniqueness of $\overline{\mathcal{P}}$ follows from the uniqueness of η_A^+ as an invariant distribution for the chain defined by transition kernel P_A on ∂A. Since $P_A(x, dy)$ satisfies the Doeblin condition (3.22), so does the chain on $\mathcal{X}$:

$$\inf_{X \in \mathcal{X}} K(X, E) \geq C^{-1} \int_{\partial A} \nu_A(dy)\mathcal{P}_y(E).$$

In particular, it is positive Harris recurrent and aperiodic, and by [26, Theorem 17.1.7], for any $\Phi \in L^1(\mathcal{X}, \mathcal{B}, \overline{\mathcal{P}})$ the limit

$$\lim_{N \to \infty} \frac{1}{N} \sum_{k=1}^{N} \Phi(X^{A,k}) = \mathbb{E}[\Phi(Z_{\cdot \wedge \tau_B}) \mid Z_0 \sim \eta_A^+] \qquad (3.25)$$

holds $\mathbb{P}$-almost surely.

Using (3.25) we will establish the following relationship between η_A^- and η_A^+:

Lemma 3.4 *Let X_t satisfy the SDE (1.1) with initial distribution $X_0 \sim \eta_A^+$ on ∂A. Then for any Borel set $U \subset \partial A$,*

$$\mathbb{P}(X_{\tau_{A,0}^-} \in U \mid X_0 \sim \eta_A^+) = \eta_A^-(U) = -\frac{1}{\nu} \int_U \rho(x)\widehat{n}(x) \cdot a(x)\nabla q(x)\, d\sigma_A(x).$$

Proof of Lemma 3.4 Let $f \in C(\mathbb{R}^d)$ be bounded and non-negative. Let us recall set S introduced in the proof of Theorem 1.2. Given $\epsilon > 0$, we let $S = \{x \in \Theta \mid q(x) < \epsilon\} \cup \overline{A}$. Then by applying (3.25) to the functional $\Phi(X) = f(X_{\tau_{S,0}^-})$, we obtain

$$\lim_{\epsilon \to 0} \lim_{N \to \infty} \frac{1}{N} \sum_{n=0}^{N-1} f(X_{\tau_{S,n}}) = \lim_{\epsilon \to 0} \mathbb{E}[f(X_{\tau_{S,0}}) \mid X_0 \sim \eta_A^+]$$

$$= \mathbb{E}[f(X_{\tau_{A,0}^-}) \mid X_0 \sim \eta_A^+].$$

We also have,

$$\lim_{N \to \infty} \frac{1}{N} \sum_{n=0}^{N-1} f(X_{\tau_{S,n}}) = \left(\lim_{K \to \infty} \frac{K}{NK} \right) \left(\lim_{K \to \infty} \frac{1}{K} \sum_{k=0}^{K-1} f(X_{r_{S,k}}) \mathbb{I}_{r_{B,k} < r_{A,k}} \right)$$

$$= \int_{\partial S} f(x) \zeta_S(dx), \tag{3.26}$$

holds $\mathbb{P}$-almost surely, where $N_K = |\{k \in \{0, 1, \dots, K-1\} \mid r_{B,k} < r_{A,k}\}|$. Here we have used ζ_S to denote the unique invariant distribution (identified below) for the Markov chain defined by $X_{r_{S,k}}$ on ∂S. Therefore,

$$\mathbb{E}[f(X_{\tau_{A,0}^-}) \mid X_0 \sim \eta_A^+] = \lim_{\epsilon \to 0} \int_{\partial S} f(x) \zeta_S(dx).$$

We claim that if $f(x)$ is uniformly continuous in a neighborhood of ∂A, then

$$\lim_{\epsilon \to 0} \int_{\partial S} \zeta_S(dx) f(x) = \int_{\partial A} \eta_A^-(dx) f(x). \tag{3.27}$$

First, let us identify the invariant distribution ζ_S. By applying Corollary 3.3 (replacing B by $\overline{S^c}$) we can identify ζ_S as

$$\zeta_S(dx) \ (= \eta_S^+(dx)) = -\frac{\epsilon}{\nu} \rho(x) \widehat{n}(x) \cdot a(x) \nabla \widetilde{q}_S(x) \, d\sigma_S(x),$$

where $\widehat{n}(x)$ is the exterior normal at $x \in \partial S$, and $\widetilde{q}_S$ satisfies $\widetilde{L} \widetilde{q}_S = 0$ in S with

$$\widetilde{q}_S(x) = \begin{cases} 1, & x \in \partial A \\ 0, & x \in \partial S. \end{cases}$$

Note that ν is independent of ϵ. Let $\delta > \epsilon$ be small, and suppose that $f(x)$ is continuous on the closed set $\{x \in \overline{\Theta} \mid 0 \le q(x) \le \delta\}$. (This set contains both ∂A and ∂S.) A computation similar to (3.12) (replacing B by S) shows that for any such function, we have

$$\int_{\partial S} \zeta_S(\mathrm{d}x) f(x) = -\frac{\epsilon}{\nu} \int_{\partial A} \rho(x)\widehat{n}(x) \cdot a(x)\nabla u_{f,S}(x)\, \mathrm{d}\sigma_A(x), \qquad (3.28)$$

where $u_{f,S}$ satisfies $Lu = 0$ in $S \backslash \overline{A}$, and

$$u_{f,S}(x) = \begin{cases} f(x), & x \in \partial S \\ 0, & x \in \partial A. \end{cases}$$

Since $f \geq 0$, we have $u > 0$ in $S \backslash \overline{A}$. Now, let us define

$$z_{f,S}(x) = \epsilon \frac{u_{f,S}(x)}{q(x)}, \quad x \in \overline{S} \backslash A,$$

which satisfies $L^q z = 0$ in $S \backslash \overline{A}$, with $z = f$ on ∂S (recall that $q(x) = \epsilon$ for all $x \in \partial S$). By the boundary Harnack inequality (see Theorem 2 and Corollary 1 of [2], as well as [5, Theorem 2.1] and [11, Theorem 11.6]), $z_{f,S}(x)$ is bounded and Hölder continuous on $\overline{S} \backslash A$ (including ∂A). We claim that for any $x_0 \in \partial A$, we have

$$\lim_{x \to x_0} \nabla u_{f,S}(x) = \epsilon^{-1} z_{f,S}(x_0) \nabla q(x_0). \qquad (3.29)$$

Since $\nabla u_{f,S}$, ∇q, and $z_{f,S}$ are continuous up to ∂A, this is true if and only if

$$\lim_{x \to x_0} q(x) \nabla z_{f,S}(x) = 0.$$

Suppose $q(x) \nabla z_{f,S}(x) \to v \neq 0$ as $x \to x_0 \in \partial A$. Then we must have

$$\lim_{x \to x_0} \nabla u_{f,S}(x) - z_{f,S}(x) \nabla q(x) = v$$

so that v must be a multiple of $\widehat{n}(x_0)$ (since u and q vanish on ∂A). Thus, we would have

$$\widehat{n}(x_0) \cdot \nabla z_{f,S}(x) \sim (\widehat{n}(x_0) \cdot v) q(x)^{-1} \qquad (3.30)$$

as $x \to x_0 \in \partial A$. If $v \neq 0$, then $(\widehat{n}(x_0) \cdot v) \neq 0$, so (3.30) and the fact that $q = 0$ on ∂A would contradict the boundedness of $z_{f,S}(x)$. Therefore, (3.29) must hold.

Combining (3.28) and (3.29) we obtain

$$\int_{\partial S} \zeta_S(\mathrm{d}x) f(x) = -\frac{1}{\nu} \int_{\partial A} \rho(x)\widehat{n}(x) \cdot a(x)\nabla q(x) z_{f,S}(x)\, \mathrm{d}\sigma_A(x) = \int_{\partial A} \eta_A^-(\mathrm{d}x) z_{f,S}(x).$$

Therefore, as $\epsilon \to 0$,

$$\lim_{\epsilon \to 0} \int_{\partial S} \zeta_S(\mathrm{d}x) f(x) = \lim_{\epsilon \to 0} \int_{\partial A} \eta_A^-(\mathrm{d}x) z_{f,S}(x) = \int_{\partial A} \eta_A^-(\mathrm{d}x) f(x). \qquad (3.31)$$

This establishes (3.27) and completes the proof of Lemma 3.4. $\qquad \square$

Now we continue with the proof of Theorem 1.7. We will apply Theorem 1.2. Suppose that $F \in L^1(\mathcal{X}, \mathcal{B}, \mathcal{Q}_{\eta_A^-})$, and define the functional

$$\Phi(X) = F(X_{(\cdot + \tau_{A,0}^-) \wedge \tau_{B,0}^+}).$$

Combining Theorem 1.2 and Lemma 3.4 we see that $\Phi \in L^1(\mathcal{X}, \mathcal{B}, \overline{\mathcal{P}})$, since

$$\begin{aligned}
\overline{\mathcal{P}}(\Phi(X) > \alpha) &= \mathbb{P}(\Phi(X) > \alpha \mid X_0 \sim \eta_A^+) \\
&= \mathbb{P}(F(X_{(\cdot + \tau_{A,0}^-) \wedge \tau_{B_0}^+}) > \alpha \mid X_0 \sim \eta_A^+) \\
&= \mathbb{Q}(F(Y) > \alpha \mid Y_0 \sim \eta_A^-) = \mathcal{Q}(F(Y) > \alpha).
\end{aligned}$$

Therefore,

$$\frac{1}{N} \sum_{k=0}^{N-1} F(Y^k) = \frac{1}{N} \sum_{k=0}^{N-1} F(X_{(\cdot + \tau_{A,k}^-) \wedge \tau_{B,k}^+}^{A,k}) = \frac{1}{N} \sum_{k=0}^{N-1} \Phi(X_\cdot^{A,k}).$$

By (3.25) and Theorem 1.2, we now conclude that the limit

$$\lim_{N \to \infty} \frac{1}{N} \sum_{k=0}^{N-1} F(Y^k) = \mathbb{E}[\Phi(Z_{\cdot \wedge \tau_B}) \mid Z_0 \sim \eta_A^+] = \widehat{\mathbb{E}}[F(Y) \mid Y_0 \sim \eta_A^-]$$

holds $\mathbb{P}$-almost surely. This completes the proof of Theorem 1.7. $\square$

4 Reaction rate, density and current of transition paths

4.1 Reaction rate

Proof of Proposition 1.8 Denote τ_B the first hitting time of X_t to $\overline{B}$. Consider the mean first hitting time

$$u_B(x) = \mathbb{E}[\tau_B \mid X_0 = x],$$

which satisfies the equation

$$\begin{cases} L u_B(x) = -1, & x \in \Theta \\ u_B(x) = 0, & x \in \partial B. \end{cases} \tag{4.1}$$

By definition of η_A^+, we have

$$\int_{\partial A} \eta_A^+(dx) u_B(x) = \frac{1}{\nu} \int_{\partial A} \rho(x) u_B(x) \widehat{n}(x) \cdot a(x) \nabla \widetilde{q}(x) \, d\sigma_A(x). \tag{4.2}$$

Observe that

$$\int_{\mathbb{R}^d} \rho(x)\widetilde{q}(x)\,dx = \int_{B^c} \rho(x)\widetilde{q}(x)\,dx$$

$$\stackrel{(4.1)}{=} -\int_{B^c} \rho(x)\widetilde{q}(x)(Lu_B)(x)\,dx$$

$$= -\int_A \rho(x)(Lu_B)(x)\,dx - \int_\Theta \rho(x)\widetilde{q}(x)(Lu_B)(x)\,dx.$$

Using (3.1) with $D = A$, $\phi(x) = 1$ and $\psi(x) = u_B$, we obtain

$$\int_A \rho(Lu_B)\,dx = -\int_{\partial A} \rho b \cdot \widehat{n} u_B \,d\sigma_A(x)$$

$$-\int_{\partial A} \rho\widehat{n} \cdot a\nabla u_B \,d\sigma_A(x) + \int_{\partial A} u_B \widehat{n} \cdot \mathrm{div}(a\rho)\,d\sigma_A(x),$$

where $\widehat{n}$ is the interior normal vector at ∂A. Apply (3.1) again with $D = \Theta$, $\phi = \widetilde{q}$ and $\psi = u_B$,

$$\int_\Theta \rho\widetilde{q}(Lu_B)\,dx = \int_{\partial A} \rho b \cdot \widehat{n} u_B \,d\sigma_A(x)$$

$$+\int_{\partial A} \rho\widehat{n} \cdot a\nabla u_B \,d\sigma_A(x) - \int_{\partial A} u_B \widehat{n} \cdot \mathrm{div}(a\rho\widetilde{q})\,d\sigma_A(x).$$

Combining the two with (4.2), we get

$$\int_{\partial A} \eta_A^+(dx)u_B(x) = \frac{1}{\nu}\int_{\partial A} \rho u_B \widehat{n} \cdot a\nabla\widetilde{q}\,d\sigma_A(x) = \frac{1}{\nu}\int_{\mathbb{R}^d} \rho\widetilde{q}\,dx.$$

Similarly, defining $u_A(x)$ to be the mean first hitting time of X_t to $\overline{A}$ starting at x, we have

$$\int_{\partial B} \eta_B^+(dx)u_A(x) = \frac{1}{\nu}\int_{\mathbb{R}^d} \rho(1-\widetilde{q})\,dx.$$

Add the integrals together to obtain

$$\int_{\partial A} \eta_A^+(dx)u_B(x) + \int_{\partial B} \eta_B^+(dx)u_A(x) = \frac{1}{\nu}.$$

On the other hand, observe that

$$\frac{1}{v_R} = \lim_{N_T \to \infty} \frac{T}{N_T}$$

$$= \lim_{N \to \infty} \frac{1}{N} \sum_{n=0}^{N-1} \left(\tau_{A,n+1}^+ - \tau_{A,n}^+ \right)$$

$$= \lim_{N \to \infty} \frac{1}{N} \sum_{n=0}^{N-1} \left(\tau_{B,n}^+ - \tau_{A,n}^+ \right) + \lim_{N \to \infty} \frac{1}{N} \sum_{n=0}^{N-1} \left(\tau_{A,n+1}^+ - \tau_{B,n}^+ \right).$$

As $N \to \infty$, we have

$$T_{AB} = \lim_{N \to \infty} \frac{1}{N} \sum_{n=0}^{N-1} \left(\tau_{B,n}^+ - \tau_{A,n}^+ \right) = \mathbb{E}[\tau_B \mid X_0 \sim \eta_A^+] = \int_{\partial A} \eta_A^+(\mathrm{d}x) u_B(x),$$

and similarly

$$T_{BA} = \lim_{N \to \infty} \frac{1}{N} \sum_{n=0}^{N-1} \left(\tau_{A,n+1}^+ - \tau_{B,n}^+ \right) = \int_{\partial B} \eta_B^+(\mathrm{d}x) u_A(x).$$

Therefore

$$\frac{1}{v_R} = \int_{\partial A} \eta_A^+(\mathrm{d}x) u_B(x) + \int_{\partial B} \eta_B^+(\mathrm{d}x) u_A(x) = \frac{1}{v},$$

or equivalently $v = v_R$.

From Theorem 1.7 it follows immediately that

$$C_{AB} = \int_{\partial A} \eta_A^-(\mathrm{d}x) v_B(x).$$

Indeed, the functional $F : Y \to \tau_B^Y$ is in $L^1(\mathcal{X}, \mathcal{B}, \mathcal{Q}_{\eta_A^-})$ by Proposition 2.7. The function $v_B(x) = \widehat{\mathbb{E}}[\tau_B^Y \mid Y_0 = x]$ satisfies

$$L^q v_B = -1, \quad x \in \Theta$$

with $v(x) = 0$ for $x \in \partial B$. Hence, the function $w(x) = q(x) v_B(x)$ satisfies $Lw = -q$ for $x \in \Theta$ with boundary condition $w(x) = 0$ for $x \in \partial \Theta$. Moreover, for $x_0 \in \partial A$, we have

$$v_B(x_0) = \lim_{x \to x_0} \frac{w(x)}{q(x)} = \frac{\widehat{n}(x_0) \cdot a(x_0) \nabla w(x_0)}{\widehat{n}(x_0) \cdot a(x_0) \nabla q(x_0)}.$$

Therefore,

$$\int_{\partial A} \eta_A^-(\mathrm{d}x) v_B(x) = -\frac{1}{\nu} \int_{\partial A} \rho(x) \widehat{n}(x) \cdot a(x) \nabla w(x) \, \mathrm{d}\sigma_A(x).$$

Now applying (3.1) with $D = \Theta$, $\phi = \tilde{q}$ and $\psi = w$, we have

$$-\frac{1}{\nu} \int_{\partial A} \rho(x) \widehat{n}(x) \cdot a(x) \nabla w(x) \, \mathrm{d}\sigma_A(x) = \frac{1}{\nu} \int_{\Theta} \rho(x) \tilde{q}(x) q(x) \, \mathrm{d}x.$$

It remains to show that

$$\nu = \int_{\mathbb{R}^d} \rho \nabla q \cdot a \nabla q \, \mathrm{d}x.$$

Using integration by parts, we have

$$\int_{\mathbb{R}^d} \rho \nabla q \cdot a \nabla q \, \mathrm{d}x = \int_{\Theta} \rho \nabla \left(q - \frac{1}{2} \right) \cdot a \nabla q \, \mathrm{d}x$$

$$= -\int_{\Theta} \nabla \cdot (\rho a \nabla q) \left(q - \frac{1}{2} \right) \mathrm{d}x + \int_{\partial A} \rho \left(q - \frac{1}{2} \right) \widehat{n} \cdot a \nabla q \, \mathrm{d}\sigma_A(x)$$

$$+ \int_{\partial B} \rho \left(q - \frac{1}{2} \right) \widehat{n} \cdot a \nabla q \, \mathrm{d}\sigma_B(x).$$

The first term on the right hand side vanishes as

$$\int_{\Theta} \nabla \cdot (\rho a \nabla q) \left(q - \frac{1}{2} \right) \mathrm{d}x = \int_{\Theta} \left(\rho \operatorname{tr} a \nabla^2 q + \rho b \cdot \nabla q \right) \left(q - \frac{1}{2} \right) \mathrm{d}x$$

$$+ \frac{1}{2} \int_{\Theta} (\operatorname{div}(\rho a) \cdot \nabla - \rho b \nabla)(q^2 - q) \, \mathrm{d}x$$

$$= \int_{\Theta} \rho(Lq) \left(q - \frac{1}{2} \right) \mathrm{d}x - \frac{1}{2} \int_{\Theta} (L^* \rho)(q^2 - q) = 0,$$

where we have used that $q^2 - q = 0$ on $\partial A \cup \partial B$. The conclusion then follows from Lemma 1.3, $q = 0$ on ∂A, and $q = 1$ on ∂B. □

4.2 Density of transition paths

We define the Green's function G_Θ of the operator L in Θ with Dirichlet boundary condition on $\partial\Theta$:

$$\begin{cases} LG_\Theta(x, y) = -\delta_y(x), & x \in \Theta, \\ G_\Theta(x, y) = 0, & x \in \partial\Theta. \end{cases} \qquad (4.3)$$

The existence of the Green's function is guaranteed by the ergodicity of X_t in $\mathbb{R}^d$, which implies that X_t is transient in Θ (see e.g. [28, Section 4.2]).

Lemma 4.1 *Let G_Θ be the Green's function of L in Θ with Dirichlet boundary condition on $\partial\Theta$. We have*

$$G_\Theta^q(x, y) \equiv \int_0^\infty Q_R(t, x, y)\, dt = \frac{q(y)G_\Theta(x, y)}{q(x)}. \qquad (4.4)$$

In particular, for $x \in \partial A,\ y \in \Theta$

$$G_\Theta^q(x, y) = \frac{q(y)\widehat{n}(x) \cdot a(x)\nabla_x G_\Theta(x, y)}{\widehat{n}(x) \cdot a(x)\nabla q(x)}. \qquad (4.5)$$

Proof Fix $y \in \Theta$. For $x \in \Theta$, (4.4) follows from [28, Proposition 4.2.2]. Specifically, the function $G_\Theta^q(x, y)$ defined by

$$G_\Theta^q(x, y) = \int_0^\infty Q_R(t, x, y)\, dt$$

is related to the Green's function (4.3) by the formula

$$G_\Theta^q(x, y) = \frac{q(y)G_\Theta(x, y)}{q(x)}, \quad x, y \in \Theta.$$

Because of the regularity of the coefficients $a(x)$ and $b(x)$, Schauder-type interior and boundary estimates imply that $G(\cdot, y) \in C^{2,\alpha}(\overline{\Theta}\backslash\{y\})$. Since $G(x, y) = q(x) = 0$ for $x \in \partial A$, the Hopf Lemma implies that for all $x \in \partial A$, $\nabla_x G(x, y)$ is a nonzero multiple of $\widehat{n}(x)$. That is, for all $x \in \partial A$, $\nabla_x G(x, y) = r(x)\widehat{n}(x)$ for some continuous $r(x) < 0$. The same is true for q. Therefore, $G_\Theta^q(x, y)$ is continuous in x up to the boundary $\partial\Theta$ and for $x_0 \in \partial A$,

$$\lim_{x \to x_0,\, x \in \Theta} G_\Theta^q(x, y) = \frac{q(y)\widehat{n}(x_0) \cdot a(x_0)\nabla_x G_\Theta(x_0, y)}{\widehat{n}(x_0) \cdot a(x_0)\nabla q(x_0)}.$$

It remains to show that for $x_0 \in \partial A$,

$$\frac{q(y)\widehat{n}(x_0) \cdot a(x_0)\nabla_x G_\Theta(x_0, y)}{\widehat{n}(x_0) \cdot a(x_0)\nabla q(x_0)} = \int_0^\infty Q_R(t, x_0, y)\, dt. \qquad (4.6)$$

Let $\varphi \geq 0$ be smooth and compactly supported in Θ. By Proposition 2.6, we have

$$\lim_{x \to x_0} \widehat{\mathbb{E}}[\varphi(Y_t) \mid Y_0 = x] = \widehat{\mathbb{E}}[\varphi(Y_t) \mid Y_0 = x_0].$$

Moreover,

$$\widehat{\mathbb{E}}[\varphi(Y_t) \mid Y_0 = x] \leq \|\varphi\|_\infty \mathbb{Q}(Y_t \in \Theta \mid Y_0 = x).$$

By Proposition 2.7, for any $R > 0$, there a function $h_R \in L^1(0, +\infty)$ such that $\mathbb{Q}(Y_t \in \Theta \mid Y_0 = x) \leq h_R(t)$ for all $x \in \Theta$, $|x| < R$, $t \geq 0$. Therefore, we have $\widehat{\mathbb{E}}[\varphi(Y_t) \mid Y_0 = x] \leq \|\varphi\|_\infty h_R(t)$ so the dominated convergence theorem implies that

$$\lim_{x \to x_0} \int_\Theta G_\Theta^q(x, y)\varphi(y) \, dy = \lim_{x \to x_0} \int_0^\infty \widehat{\mathbb{E}}[\varphi(Y_t) \mid Y_0 = x] \, dt$$

$$= \int_0^\infty \widehat{\mathbb{E}}[\varphi(Y_t) \mid Y_0 = x_0] \, dt$$

$$= \int_0^\infty \left(\int_\Theta Q(t, x_0, y)\varphi(y) \, dy \right) dt. \quad (4.7)$$

On the other hand, we also have

$$\lim_{x \to x_0} \int_\Theta G_\Theta^q(x, y)\varphi(y) \, dy = \int_\Theta \frac{q(y)\widehat{n}(x_0) \cdot a(x_0)\nabla_x G_\Theta(x_0, y)}{\widehat{n}(x_0) \cdot a(x_0)\nabla q(x_0)} \varphi(y) \, dy. \quad (4.8)$$

Therefore, by combining (4.7) and (4.8) we conclude

$$\int_\Theta \frac{q(y)\widehat{n}(x_0) \cdot a(x_0)\nabla_x G_\Theta(x_0, y)}{\widehat{n}(x_0) \cdot a(x_0)\nabla q(x_0)} \varphi(y) \, dy = \int_0^\infty \int_\Theta Q(t, x_0, y)\varphi(y) \, dy \, dt$$

$$= \int_\Theta \left(\int_0^\infty Q(t, x_0, y) \, dt \right) \varphi(y) \, dy.$$

Since φ is arbitrary, this implies (4.6). $\qquad \square$

Proof of Proposition 1.9 Using Lemma 4.1 and (1.38),

$$\rho_R(z) = \nu_R \int_{\partial A} \eta_A^-(dx) G_\Theta^q(x, z). \quad (4.9)$$

Recall the explicit formula of η_A^- in terms of q (1.23), we obtain for $z \in \Theta$

$$\rho_R(z) = -\int_{\partial A} \rho(x) \frac{q(y)\widehat{n}(x) \cdot a\nabla_x G_\Theta(x,z)}{\widehat{n}(x) \cdot a\nabla q(x)} \widehat{n}(x) \cdot a\nabla q(x) \, d\sigma_A(x)$$

$$= -q(y) \int_{\partial A} \rho(x)\widehat{n}(x) \cdot a\nabla_x G_\Theta(x,z) \, d\sigma_A(x).$$

Apply (3.1) by taking $\psi(x) = G_\Theta(x,y)$ and $\phi(x) = \widetilde{q}(x)$, we conclude that

$$\rho_R(y) = -q(y) \int_{\partial \Theta} \rho(x)\phi(x)\widehat{n}(x) \cdot a\nabla\psi(x) \, d\sigma_\Theta(x)$$

$$= -q(y) \int_\Theta \rho(x)\phi(x)L\psi(x)$$

$$= \rho(y)q(y)\widetilde{q}(y).$$

Here to get the second equality, we have used that $\widetilde{L}\widetilde{q} = 0$ in Θ and $\psi(x) = 0$ on $\partial\Theta$. $\qquad\square$

4.3 Current of transition paths

Proof of Proposition 1.10 It follows from a direct calculation from the definition of J_R as (1.41), noticing that $q = 0, \widetilde{q} = 1$ on ∂A, and $q = 1, \widetilde{q} = 0$ on ∂B. $\qquad\square$

Proof of Corollary 1.11 By Proposition 1.10, we have

$$v_R = -\int_{\partial A} \widehat{n}(x) \cdot J_R(x) \, d\sigma_A(x).$$

Hence, it suffices to show that

$$\int_{\partial A} \widehat{n}(x) \cdot J_R(x) \, d\sigma_A(x) + \int_{\partial S} \widehat{n}(x) \cdot J_R(x) \, d\sigma_S(x) = 0,$$

which follows from the fact that J_R is divergence free in Θ (see (1.40)). $\qquad\square$

Proof of Proposition 1.12 Using Proposition 1.10 for the left hand side of (1.45), we obtain

$$\int_{\partial B} f(x)\eta_B^+(dx) - \int_{\partial A} f(x)\eta_A^-(dx) = \frac{1}{v_R}\int_{\partial B} f\widehat{n} \cdot J_R \, d\sigma_B + \frac{1}{v_R}\int_{\partial A} f\widehat{n} \cdot J_R \, d\sigma_A,$$

where $\widehat{n}$ is the unit normal exterior to Θ. Equation (1.45) then follows from the divergence theorem.

Now fix any $g \in C^1(\partial B)$, we extend g to $\overline{\Theta}$ using the flow (1.43): for any $x \in \overline{\Theta}$, we define

$$g(x) = g(Z^x_{t_B}), \quad \text{with } Z^x_0 = x. \tag{4.10}$$

In particular, for $x \in \partial A$, we have $g(x) = g(\Phi_{J_R}(x))$, in other words,

$$g|_{\partial A} = \Phi^*_{J_R}(g|_{\partial B}). \tag{4.11}$$

By the construction (4.10), for any $x \in \Theta$, $J_R \cdot \nabla g = 0$. Combining with the first part of the Proposition and (4.11), we obtain

$$\int_{\partial B} g(x) \eta^+_B(\mathrm{d}x) = \int_{\partial A} \Phi^*_{J_R} g \, \eta^-_A(\mathrm{d}x).$$

Therefore, $\Phi_{J_R,*}(\eta^-_A) = \eta^+_B$.

References

1. Athreya, S.R., Barlow, M.T., Bass, R.F., Perkins, E.A.: Degenerate stochastic differential equations and super-Markov chains. Probab. Theory Relat. Fields **123**, 484–520 (2002)
2. Athanasopoulos, I., Caffarelli, L.A.: A theorem of real analysis and its application to free boundary problems. Commun. Pure Appl. Math. **38**, 499–502 (1985)
3. Athreya, K.B., Ney, P.: A new approach to the limit thoery of recurrent markov chains. Trans. Am. Math. Soc. **245**, 493–501 (1978)
4. Bakhtin, Y.: Gumbel distribution in exit problems (2013, preprint) [arXiv:1307.7060]
5. Bauman, P.: Positive solutions of elliptic equations in nondivergence form and their adjoints. Ark. Mat. **22**, 153–173 (1984)
6. Bolhuis, P.G., Chandler, D., Dellago, C., Geissler, P.L.: Transition path sampling: throwing ropes over rough mountain passes, in the dark. Annu. Rev. Phys. Chem. **53**, 291–318 (2002)
7. Bovier, A., Eckhoff, M., Gayrard, V., Klein, M.: Metastability in reversible diffusion processes I. Sharp asymptotics for capacities and exit times. J. Eur. Math. Soc. **6**, 399–424 (2004)
8. Bovier, A., Gayrard, V., Klein, M.: Metastability in reversible diffusion processes II. Precise asymptotics for small eigenvalues. J. Eur. Math. Soc. **7**, 69–99 (2005)
9. Berman, K.A., Konsowa, M.H.: Random paths and cuts, electrical networks, and reversible Markov chains. SIAM J. Discrete Math. **3**, 311–319 (1990)
10. Cerou, F., Guyader, A., Lelievre, T., Malrieu, F.: On the length of one-dimensional reactive paths (2012, preprint) [arXiv:1206.0949]
11. Caffarelli, L., Salsa, S.: Geometric Approach to Free Boundary Problems. American Mathematical Society, Providence (2005)
12. Dellago, C., Bolhuis, P.G., Geissler, P.L.: Transition path sampling. Adv. Chem. Phys. **123** (2002)
13. Dean, T., Dupuis, P.: The design and analysis of a generalized RESTART/DPR algorithm for rare event simulation. Ann. Oper. Res. **189**, 63–102 (2011)
14. DeBlassie, D.: Uniqueness for diffusions degenerating at the boundary of a smooth bounded set. Ann. Probab. **32**, 3167–3190 (2004)
15. Weinan, E., Vanden-Eijnden, E.: Toward a theory of transition paths. J. Stat. Phys. **123**, 503–523 (2006)
16. Weinan, E., Vanden-Eijnden, E.: Transition path theory and path-finding algorithms for the study of rare events. Annu. Rev. Phys. Chem. **61**, 391–420 (2010)
17. Freidlin, M.I., Wentzell, A.D.: Random Perturbations of Dynamical Systems. Springer, Berlin (1984)
18. Gilberg, D., Trudinger, N.S.: Elliptic Partial Differential Equations of Second Order. Springer, Berlin (1998)

19. Haussmann, U.G., Pardoux, É.: Time reversal of diffusions. Ann. Probab. **14**, 1188–1205 (1986)
20. Hairer, M., Stuart, A.M., Voss, J.: Analysis of SPDEs arising in path sampling part II: the nonlinear case. Ann. Appl. Probab. **17**, 1657–1706 (2007)
21. Hairer, M., Stuart, A.M., Voss, J., Wiberg, P.: Analysis of SPDEs airisng in path sampling part I: the Gaussian case. Commun. Math. Sci. **3**, 587–603 (2005)
22. Hummer, G.: From transition paths to transition states and rate coefficients. J. Chem. Phys. **120**, 516–523 (2004)
23. Karatzas, I., Shreve, S.: Brownian Motion and Stochastic Calculus, 2nd edn. Springer, New York (1991)
24. Metzner, P., Schütte, C., Vanden-Eijnden, E.: Illustration of transition path theory on a collection of simple examples. J. Chem. Phys. **125**, 084110 (2006)
25. Meyer, P.A., Smythe, R.T., Walsh, J.B.: Birth and death of markov processes. In: Proceedings of the Sixth Berkeley Symposium on Mathematical Statistics and Probability, Vol. III, pp. 295–305 (1972)
26. Meyn, S.P., Tweedie, R.L.: Markov Chains and Stochastic Stability, 2nd edn. Cambridge University Press, Cambridge (2009)
27. Prinz, J.-H., Held, M., Smith, J.C., Noé, F.: Efficient computation, sensitivity, and error analysis of committor probabilities for complex dynamical processes. Multiscale Model. Simul. **9**, 545–567 (2011)
28. Pinsky, R.G.: Positive Harmonic Functions and Diffusion, Cambridge Studies in Advanced Mathematics, vol. 45. Cambridge University Press, Cambridge (1995)
29. Reznikoff, M.G., Vanden-Eijnden, E.: Invariant measures of stochastic partial differential equations and conditioned diffusions. C. R. Acad. Sci. Paris Ser. I **340**, 305–308 (2005)
30. Revuz, D., Yor, M.: Continuous Martingales and Brownian Motion. Springer, New York (1999)
31. Stuart, A.M., Voss, J., Wiberg, P.: Conditional path sampling of SDEs and the Langevin MCMC method. Commun. Math. Sci. **2**, 685–697 (2004)
32. Sznitman, A.-S.: Brownian Motion, Obstacles and Random Media. Springer, New York (1998)
33. Vanden-Eijnden, E.: Transition path theory (2013, preprint)
34. Veretennikov, A.Yu.: On polynomial mixing bounds for stochastic differential equations. Stochastic Process Appl. **70**, 115–127 (1997)
35. Vanden-Eijnden, E., Venturoli, M., Ciccotti, G., Elber, R.: On the assumptions underlying milestoning. J. Chem. Phys. **129**, 174102 (2008)
36. Vanden-Eijnden, E., Weare, J.: Rare event simulation of small noise diffusions. Commun. Pure Appl. Math. **65**, 1770–1803 (2012)