METASTABILITY OF DIFFUSION PROCESSES

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Abstract Diffusion models arising in analysis of real world systems are typically far too complex for exact solution, or even meaningful simulation. The purpose of this paper is to develop foundations for model reduction, and new modeling techniques for diffusion models. Based on the main assumption of V*-uniform ergodicity* of the diffusion process it is shown that real eigenfunctions provide a decomposition of the state space into so-called metastable sets. We give a novel definition of metastability via exit rates which seems to be promising for a algorithmic identification of metastable sets even for large scale systems.

Introduction

Diffusion models are a popular alternative to the classical description of complex processes in terms of large sets of ordinary differential equations that give rise to chaotic dynamics. Examples are varied and come from the such diverse fields as molecular dynamics [4], materials science [5], or internet security [3]. However, even diffusion models in practice are far too complex for exact solution, or even long-term simulation.

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Recently, various approaches to the essential features of such diffusion models have been proposed. They range from novel algorithmic methods based on transfer operator theory that decompose the state space into 'metastable' sets [16, 17] and transition path computation between these sets [6, 4], to more theoretical approaches to model reduction techniques based on variants of the classical Wentzell–Freidlin theory (see e.g. [2, 7, 15]), or the analysis of transition times via the theory of quasi-stationary distributions of Markov process as introduced in [18, 19, 8]. The approaches closest to this article are [2, 7]. However, while the present article defines and investigates the essential features of diffusion processes via resent results for spectral theory, [7] mainly exploits large deviation theory and [2] is mainly concerned with the limit of vanishing noise intensity (which is not the case in the present article).

The approach via quasi-stationary distributions and the mentioned algorithmic transfer operator approach, both, rely on the analysis of eigenfunctions of the full or some restricted semigroup of the diffusion process. This article corresponds to this discussion, combined with recent results concerning large deviations and spectral theory for ψ-irreducible Markov processes [1, 10, 11]. It summarizes the article [9] of the present authors. There, the theory is worked out in detail, while we here aim to provide a rapidly accessible reference to the results in [9] combined with a short nontrivial illustration.

We consider general multivariate diffusion processes $\boldsymbol{X}$ which are governed by the stochastic differential equation

$$\mathrm{d}X \quad = \quad u(X)\,\mathrm{d}t + A(X)\,\mathrm{d}W,, \tag{1}$$

where $u : \mathbb{R}^d \to \mathbb{R}^d$ with measurable components, W denotes d-dimensional Brownian motion, and $A(x)$ a $d \times d$ matrix with measurable entries. A special case is the so-called Smoluchowski or high friction Langevin equation on $\mathbb{R}^d$, where the function u is given by a potential U, $u = -\nabla U$, and the matrix A is state-independent and a multiple of the identity matrix, $A = \sigma I$, such that the process obeys $\mathrm{d}X = -\nabla U(X)\,\mathrm{d}t + \sigma\,\mathrm{d}W,$. Choosing $d = 1$ and U to be the perturbed three well potential shown in Figure 1, we will use this case for illustration.

1. V-uniform ergodicity and spectral gaps

Here we assume that the reader is acquainted with the basics of the general theory of Markov processes, especially with the definitions of ψ-irreducibility, (Harris) recurrence, and aperiodicity. The state space $\mathbb{X}$ considered herein is assumed to be an open, connected subset of $\mathbb{R}^d$. The ergodic theory and spectral theory described here is based upon the vector space setting developed in [12, Chapter 16]. Let $V : \mathbb{X} \to [1, \infty)$

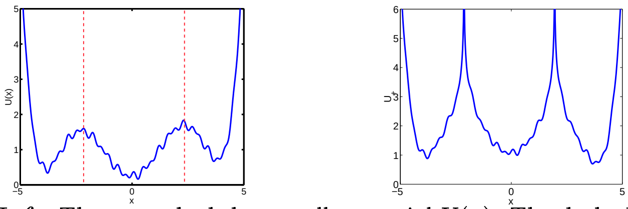

Figure 1. Left: The perturbed three–well potential $U(x)$. The dashed lines indicate the wells separated by the two saddle points with maximal barriers. Right: Corresponding potential of the so-called twisted process due to Prop. 4 below based on the eigenfunction h_3 of our illustrative example (see Figure 2, middle).

be a given function, and denote by L_∞^V the vector space of measurable functions $h: \mathbb{X} \to \mathbb{C}$ satisfying

$$\|h\|_V := \sup_{x \in \mathbb{X}} \frac{|h(x)|}{V(x)} < \infty.$$

The vector space $\mathcal{M}_1^V$ is the set of complex-valued measures ν on the Borel sigma-field $\mathcal{B} = \mathcal{B}(\mathbb{X})$ such that

$$\|\nu\|_V := \int_{\mathbb{X}} V(x)|\nu(dx)| < \infty.$$

The induced operator norm is defined by

$$|\!|\!|P|\!|\!|_V := \sup \frac{\|Ph\|_V}{\|h\|_V},$$

where the supremum is over $h \in L_\infty^V$, $\|h\|_V \neq 0$. For later reference, we define the function space

$$C^V = \{g \in L_\infty^V : \|P^t g - g\|_V \to 0,\ t \downarrow 0\}.$$

1.1 Diffusion semigroups

Based on the previous definitions this section will present some spectral theory for the semigroup associated with a hypoelliptic diffusion process: We assume that time is continuous, $\mathbb{T} := \mathbb{R}_+$, and that the diffusion $\boldsymbol{X} = \{X(t) : t \in \mathbb{T}\}$ evolves on $\mathbb{X}$ due to (1). Its differential generator (the generator of the associated Fokker-Planck equation) is given by

$$\mathcal{D}h = \sum_i u_i(x) \frac{\partial}{\partial x_i} h(x) + \tfrac{1}{2} \sum_{ij} \Sigma_{ij}(x) \frac{\partial^2}{\partial x_i \partial x_j} h(x) \qquad (2)$$

with $\Sigma_{ij}(x)$ being the entries of the $d \times d$ matrix $\Sigma(X) = A(x)A(x)^T$. In more compact notation, $\mathcal{D} = -u \cdot \nabla + \frac{1}{2}\mathrm{trace}\,(\Sigma\nabla^2)$. In the following we assume that

$$\text{\textit{the Markov process } } \boldsymbol{X} \text{ \textit{is an aperiodic, hypoelliptic diffusion, with continuous sample paths.}} \tag{3}$$

The definition of hypoellipticity can be found, e.g., in [13, Theorem 3.3]. The following theorem gives a condition under which this assumption holds:

Theorem 1 *Suppose that $\boldsymbol{X}$ is a diffusion with generator given in (2), and suppose that the generator is hypoelliptic. Suppose moreover that there is a state $x_0 \in \mathbb{X}$ that is 'reachable' in the following sense: For any $x \in \mathbb{X}$, and any open set O whose closure contains x_0, we have that $P^t(x, O) > 0$, for all $t \in \mathbb{T}$ sufficiently large. Then, the Markov process is ψ-irreducible and aperiodic with*

$$\psi(\cdot) \quad = \quad \int_0^\infty e^{-t} P^t(x_0, \cdot)\,\mathrm{d}t. \tag{4}$$

The RHS of (4) is know as the resolvent kernel corresponding to the transition function P^t of the diffusion defined in (1). Formulations and characterizations of the *spectral gap* of our diffusion $\boldsymbol{X}$ are facilitated by three different **generators**:

1 The *extended generator* $\mathcal{A}$: We write $g = \mathcal{A}f$ if the adapted stochastic process $(M_f(t), \mathcal{F}_t)$ is a local martingale, where $\mathcal{F}_t = \sigma(X(s); 0 \le s \le t)$, and

$$M_f(t) := f(X(t)) - f(X(0)) - \int_0^t g(X(s))\,\mathrm{d}s\,. \tag{5}$$

2 The *differential generator* $\mathcal{D}$: Defined on $C^2(\mathbb{X})$ via $\mathcal{D}f = -u \cdot \nabla f + \frac{1}{2}\mathrm{trace}\,(\Sigma\nabla^2 f)$.

3 The *strong generator* $\mathcal{D}_V$: For a given $V\colon \mathbb{X} \to [1, \infty]$, finite a.e., we write $g = \mathcal{D}_V f$ if $f, g \in C^V$, and $\|\frac{P^t f - f}{t} - g\|_V \to 0$ for $t \downarrow 0$.

The extended generator $\mathcal{A}$ is a true extension of $\mathcal{D}$ in the sense that $\mathcal{A}f = \mathcal{D}f$ a.e. $[\psi]$ when $f \in C^2(\mathbb{X})$. The extended generator and differential generator are used in criteria for stability and to obtain bounds on the 'essential spectrum' of the associated semigroup. The strong generator is used to define a **spectral gap**: For a given $V\colon \mathbb{X} \to [1, \infty]$, finite a.e., 1 The *spectrum* $\mathrm{s}(\mathcal{D}_V)$ is the set of $\Lambda \in \mathbb{C}$ such that the inverse $[I\Lambda - \mathcal{D}_V]^{-1}$ does not exist as a bounded linear operator on L_∞^V;

2 The generator admits a *spectral gap* if the set $\mathrm{s}(\mathcal{D}_V) \cap \{z \in \mathbb{C} : \mathrm{Re}(z) \geq -\varepsilon\}$ is finite for sufficiently small $\varepsilon > 0$;

3 The Markov process is called *V-uniformly ergodic* if there is a spectral gap; $\{0\} = \mathrm{s}(\mathcal{D}_V) \cap \{z \in \mathbb{C} : \mathrm{Re}(z) = 0\}$; and the eigenvalue $\Lambda = 0$ is simple.

The following 'drift condition' characterizes V-uniform ergodicity and is central to this paper. It is useful that we may use the extended generator, and not the strong generator in (V4). A function $s\colon \mathbb{X} \to [0,\infty)$ is called *small* if

$$P^T(x,A) \geq \varepsilon s(x)\nu(A), \qquad x \in \mathbb{X}.$$

for some probability distribution ν on $\mathcal{B}(\mathbb{X})$, $\varepsilon > 0$, and $T < \infty$.

(V4) *For constants $b < \infty$, $0 < \overline{\Gamma} < \infty$, a small function $s : \mathbb{X} \to [0,\infty)$, and a function $V : \mathbb{X} \to [1,\infty)$, one has $\mathcal{A}V \leq -\overline{\Gamma}V + bs$.*

Condition (V4) is equivalent only to a spectral gap.

Theorem 2 *Suppose that $\boldsymbol{X}$ is ψ-irreducible and aperiodic, and suppose that (V4) holds for some $V\colon \mathbb{X} \to [1,\infty)$. Then $\boldsymbol{X}$ is V-uniformly ergodic. Conversely, if the Markov process $\boldsymbol{X}$ is V_0-uniformly ergodic then there exists a solution to (V4) with $V \in L_\infty^{V_0}$.*

1.2 Non–probabilistic semigroups

For a given function $F\colon \mathbb{X} \to \mathbb{R} \cup \{\infty\}$ we consider the following *positive semigroup*, for $A \in \mathcal{B}, x \in \mathbb{X}, t \in \mathbb{T}$,

$$P_F^t(x,A) = \mathsf{E}_x\Big[\mathbf{1}(X(t) \in A)\exp\Big(-\int_0^t F(X(s))\,\mathrm{d}s\Big)\Big].$$

A strong generator can be defined in analogy with the probabilistic semigroup.

For an arbitrary positive semigroup $\{\widehat{P}^t\}$ the definitions of irreducibility, small sets and measures, and other set classifications remain the same in this non-probabilistic setting. For a given function $V\colon \mathbb{X} \to [1,\infty]$, finite a.e., the *$V$-spectral radius* of $\{\widehat{P}^t\}$ is given by

$$\mathrm{sr}_V(\{\widehat{P}^t\}) := \lim_{T\to\infty} \Big(|||\widehat{P}^T|||_V\Big)^{1/T}.$$

Closely related is the *Perron-Frobenius eigenvalue*, defined for any small pair (s,ν) with $s \in \mathcal{B}^+$, $\nu \in \mathcal{M}^+$, via

$$\mathrm{pfe}(\{\widehat{P}^t\}) \;:=\; \lim_{T\to\infty}\Big(\nu \widehat{P}^T s\Big)^{1/T} \tag{6}$$

A straightforward generalization of [14, Proposition 3.4] shows that these definition are independent of the particular small pair chosen when the process is ψ-irreducible.

In analogy with V-uniform ergodicity, the semigroup $\{\widehat{P}^t : t \in \mathbb{R}_+\}$ with generator $\widehat{\mathcal{D}}_V$ is called *V-uniform* if the following conditions are satisfied:

1 The constant $\Lambda := -\log(\mathrm{sr}_V(F))$ is a *simple eigenvalue*, i.e., the associated eigenspace is a one-dimensional subspace of L^V_∞.

2 The generator admits spectral gap: for sufficiently small $\varepsilon > 0$,

$$\{\Lambda\} = \mathrm{s}(\widehat{\mathcal{D}}_V) \cap \{z \in \mathbb{C} : \mathrm{Re}(z) \geq \Lambda - \varepsilon\}\,.$$

In [9], the reader may find an analog of Theorem 2 which states the V-uniformity of the semigroup $\{\widehat{P}^t_F\}$ under the assumption of a drift condition similar to (V4).

2. Metastability and exit rates

For a given set $A \in \mathcal{B}$ we define the stopping times,

$$\tau_A := \inf\Big\{t > 0 : X(t) \in A\Big\},\; \varrho_A := \inf\Big\{t > 0 : \int_0^t \mathbf{1}(X(s) \in A)\,\mathrm{d}s > 0\Big\}$$

Much of the analysis here is based on the semigroups $\{\widehat{P}^t_F\}$ considered in Section 1.2 in the special case where $F = \infty\mathbf{1}_{A^c}$ for some $A \in \mathcal{B}$. When F takes this form we denote the semigroup by $\{\widehat{P}^t_A\}$, which can be equivalently expressed,

$$P^t_A g\,(x) = \mathsf{E}_x[g(X(t))\mathbf{1}(\varrho_{A^c} \geq t)], \qquad g \in L_\infty,\; x \in \mathbb{X},\; t \in \mathbb{T}\,.$$

Let $\mathcal{C}$ denote the collection of all connected, open subsets of $\mathbb{X}$. In addition to assumption (3) the following assumptions will be imposed throughout the subsequent:

For each $A \in \mathcal{C}$ the semigroup $\{P^t_A\}$ is ψ_A-irreducible, where ψ_A is Lebesgue measure restricted to A, and every compact subset of A is a small set for $\{P^t_A\}$. (7)

2.1 Exit rates

Our goal in this section is to quantify the rate at which the process moves between elements of $\mathcal{C}$. The motivation for the consideration of transition *rates*, rather than moments, is to set the stage for Markov chain approximations. **Exit rates and metastable sets** are defined as follows

1 The *exit rate* of $A \in \mathcal{C}$ is defined as $\Gamma(A) := -\log(\text{pfe}(A))$, where $\text{pfe}(A)$ denotes the Perron-Frobenius eigenvalue for the semigroup $\{P_A^t : t \in \mathbb{T}\}$ as defined in eq. (6).

2 A set $\mathsf{M} \in \mathcal{C}$ is called *metastable* with exit rate $\Gamma(\mathsf{M})$ if $\Gamma(A) > \Gamma(\mathsf{M})$ for all $A \subset \mathsf{M}$, $A \neq \mathsf{M}$, $A \in \mathcal{C}$.

3 The *V-exit rate* of $A \in \mathcal{B}$ is given by $\Gamma_V(A) := -\log(\text{sr}_V(A))$, where $\text{sr}_V(A)$ denotes the V-spectral radius of $\{P_A^t\}$.

4 For $\mathsf{M} \in \mathcal{B}$ we say that M is *V-metastable* if $\Gamma_V(\mathsf{M}) < \infty$, and $\Gamma_V(A) > \Gamma_V(\mathsf{M})$ for any $A \subset \mathsf{M}$ satisfying $A \in \mathcal{B}$ and $\psi(\mathsf{M}/A) > 0$.

Certain metastable sets are closely related to eigenfunctions:

Theorem 3 *Suppose that $\boldsymbol{X}$ is a diffusion satisfying (3) and (7), and that $\mathsf{M} \in \mathcal{C}$ is both metastable and V-metastable, with common exit rate $\Gamma(\mathsf{M}) = \Gamma_V(\mathsf{M}) < \infty$. Then there exists $h \colon \mathsf{M} \to (0, \infty)$ satisfying the eigenvalue equation*

$$\mathcal{A}h = -\Gamma(\mathsf{M})h \qquad \text{on } \mathsf{M}. \tag{8}$$

Here, for a set $A \in \mathcal{C}$ and functions $f, g \colon A \to \mathbb{R}$ we write '$g = \mathcal{A}f$ *on* A' if $\{M_f(t \wedge \varrho_{A^c}) : t \in \mathbb{T}\}$ is a local martingale (see (5)).

2.2 The twisted process

Inspired by Theorem 3, this section investigates the consequences of the following **eigenfunction equation**:

For some $\Gamma_0 < \infty$ and some set $\mathsf{M} \in \mathcal{C}$ there exists a function h, positive on M and C^2 in a neighborhood of $\bar{\mathsf{M}}$ such that $\mathcal{D}h\,(x) = -\Gamma_0 h(x)$, for $x \in \mathsf{M}$. (9)

Under (9), for any $x \in \mathbb{X}$ the stochastic process $m_h(t) := h(x)^{-1} h(X(t)) e^{\Gamma_0 t}$, $t \in \mathbb{T}$, is a positive martingale up to the stopping time $T_\bullet := \varrho_{\mathsf{M}^c}$. Hence it may serve in a change of measure in the construction of the **twisted process** $\check{\boldsymbol{X}}$ with state space $\check{\mathbb{X}} := \mathsf{M}$ whose semigroup is defined for any $g \in L_\infty(\mathsf{M})$, and any $x \in \mathsf{M}$ via,:

$$\check{\mathsf{E}}_x[g(\check{X}(t))] := \mathsf{E}_x[m_h(t) g(X(t)) \mathbf{1}(T_\bullet > t)]\,. \tag{10}$$

The twisted process is a diffusion. The associated 'twisted generator' is given in Proposition 4 below.

Proposition 4 *Suppose that (3), (7) and (9) hold. Then, The expectation operator $\check{\mathsf{E}}$ defines a diffusion on M, up to the exit time $T_\bullet$. The differential generator is given by,*

$$\check{\mathcal{D}} = I_{h^{-1}}\mathcal{D}I_h + \Gamma_0 I \;=\; \mathcal{D} + \langle \Sigma(\nabla H), \nabla\rangle, \tag{11}$$

where I_h is the multiplication operator: $I_h g = h{\cdot}g$, and $H(x) = \log(h(x))$ for $x \in \mathsf{M}$. If $\boldsymbol{X}$ is governed by a Smoluchowski equation on $\mathbb{X}$ with potential U, and if $\Sigma = \sigma^2 I$, then $\check{\mathcal{D}}$ is the differential generator for a Smoluchowski equation with potential $U_+ = U - \sigma^2 H$.

The following result characterizes metastability in terms of geometric ergodicity of the twisted process.

Theorem 5 *Assume that (3), (7) and (9) hold. Suppose moreover that the escape-time for the twisted process is infinite a.s., and that the twisted process is $\check{V}$-uniformly ergodic for some $\check{V}\colon \mathsf{M} \to [1,\infty)$, with $h^{-1} \in L_\infty^{\check{V}}$. Then, the set M is both metastable and V_0-metastable, with common exit rate $\Gamma(\mathsf{M}) = \Gamma_{V_0}(\mathsf{M}) = \Gamma_0$ given in (9), and with $V_0 = \check{V}h$.*

We now provide more readily verifiable sufficient conditions under which the conclusions of Theorem 5 will hold.

Theorem 6 *Assume that (3), (7) and (9) hold, and that (V4) is also satisfied for a continuous function $V\colon \mathbb{X} \to [1,\infty)$. Suppose moreover that the Lyapunov function V and the eigenfunction h satisfy the following additional conditions:*

(a) *The constant Γ_0 in (9) satisfies $0 < \Gamma_0 < \overline{\Gamma}$.*

(b) *$h(x) > 0$ for all $x \in \mathsf{M}$, and $h(x) = 0$ for $x \in \partial\mathsf{M} := \bar{\mathsf{M}} \setminus \mathsf{M}$.*

(c) *$(\nabla h(x))^{\intercal}\Sigma(x)(\nabla h(x)) > 0$ for all $x \in \partial\mathsf{M}$.*

(d) *$K_n := \{x \in \mathbb{X} : V(x) \le n h(x)\}$ is a compact subset of $\mathbb{X}$ for all $n \ge 1$.*

Then,

(i) *The escape-time from M for the twisted process is infinite a.s. for $\check{X}(0) = x \in \mathsf{M}$;*

(ii) *The twisted process is $\check{V}_1$-uniformly ergodic with $\check{V}_1 = V/h$.*

(iii) *The set M is both metastable and V-metastable, with exit rate $\Gamma(\mathsf{M}) = \Gamma_V(\mathsf{M}) = \Gamma_0$, where Γ_0 is given in (9).*

The following data illustrates the meaning of Theorem 6 for the Smoluchowski equation $\mathrm{d}X = -\nabla U(X)\,\mathrm{d}t + \sigma\,\mathrm{d}W$ in dimension $d = 1$ with the perturbed three well potential U of Figure 1 and $\sigma = 1$. The eigenproblem of the generator has been solved numerically by means of an appropriate finite element solver. The resulting eigenvalues are:

λ_1	λ_2	λ_3	λ_4	λ_5	...
0.000	−0.041	−0.069	−0.906	−1.419	...

Thus, the eigenfunctions associated with the low eigenvalues λ_2 and λ_3 should allow a decomposition of state space into metastable sets with significantly small exit rates. This eigenfunctions are shown in Figure 2. We observe that the decompositions based on the zeros of the eigenfunctions h_2 or h_3, respectively, are related to the decomposition into the three dominant wells of the potential; deviations of the zeros from the location of the saddle points with maximal barriers are in detail discussed in [9].

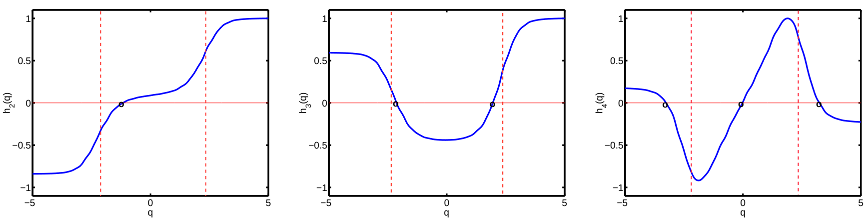

Figure 2. Second to forth eigenfunction $h_2, \ldots, h_4$ of the generator for the Smoluchowski equation with the perturbed three–well potential and $\sigma = 1$. The first eigenfunction h_1 is constant. The dashed lines indicate the main wells of the potential as in Figure 1. Note that the eigenfunctions are remarkable insensitive to large variations of the potential function.

2.3 Consequences for exit times

We show here that $\check{V}$-uniform ergodicity of the twisted process implies that the exit time $T_\bullet := \varrho_{\mathsf{M}^c}$ from a metastable set M is approximately exponentially distributed, with rate $\Gamma(\mathsf{M})$, provided there is a sufficient spectral gap. For the random variable $T_\bullet$ we define the conditional distribution function, and the conditional moment generating function for the residual life at time T by

$$\begin{aligned} F_x(s,T) &= \mathsf{P}_x[(T_\bullet - T) \geq s \mid T_\bullet \geq T], \qquad s \geq 0,\ T \geq 0; \\ M_x(\beta,T) &= \mathsf{E}_x[\exp(\beta(T_\bullet - T)) \mid T_\bullet \geq T], \quad \beta \leq \Gamma,\ T \geq 0\,. \end{aligned} \tag{12}$$

These quantities are independent of T only for exponential random variables. Theorem 7 states that the rate of decay of the exit time is basically independent of the starting point and of T.

Theorem 7 *Suppose that the conditions of Theorem 6 hold, so that the set* M *is* V*-metastable with exit-rate* $\Gamma > 0$*. Then there exists* $\delta_0 > 0$ *such that for all* $s, T > 0$ *and all* $\beta < \Gamma$*,*

$$\begin{aligned} F_x(s,T) &= e^{-\Gamma s}\left[\frac{1+O\left(e^{-\delta_0 s}V(x)h^{-1}(x)\right)}{1+O\left(e^{-(T+s)\delta_0}V(x)h^{-1}(x)\right)}\right] \\ M_x(\beta,T) &= \frac{\Gamma}{\Gamma-\beta} + O\left(e^{-\delta_0 T}V(x)h^{-1}(x)\right) \end{aligned}$$

Under the conditions supposed here, an application of Theorem 6 implies that the twisted process is $\check{V}$-uniformly ergodic for some $\check{V}$ satisfying $h^{-1} \in L_\infty^{\check{V}}$. It follows that, for some $\delta_0 > 0$,

$$\check{P}^s h^{-1}(x) = \check{\pi}(h^{-1}) + O(e^{-\delta_0 s}V(x)h^{-1}(x)) \quad s \geq 0,\ x \in \mathbb{X}. \qquad (13)$$

Exacty this δ_0 is the constant that enters in Theorem 7. The potential for the twisted process(es) based on the eigenfunction h_3 of our illustrative example is shown in Figure 1. In each of the three parts the twisted potential does not exhibit any significant barriers. Thus, the diffusion is rapidly mixing in all three components and therefore the associated δ_0 is large compared to the low eigenvalues of the full spectrum.

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