Hypocoercivity of Piecewise Deterministic Markov Process-Monte Carlo

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Abstract

In this work, we establish L^2-exponential convergence for a broad class of Piecewise Deterministic Markov Processes recently proposed in the context of Markov Process Monte Carlo methods and covering in particular the Randomized Hamiltonian Monte Carlo [21, 11], the Zig-Zag process [6] and the Bouncy Particle Sampler [51, 12]. The kernel of the symmetric part of the generator of such processes is non-trivial, and we follow the ideas recently introduced in [20, 21] to develop a rigorous framework for hypocoercivity in a fairly general and unifying set-up, while deriving tractable estimates of the constants involved in terms of the parameters of the dynamics. As a by-product we characterize the scaling properties of these algorithms with respect to the dimension of classes of problems, therefore providing some theoretical evidence to support their practical relevance.

1 Introduction

Consider a probability distribution π defined on the Borel σ-field $\mathcal{X}$ of some domain $\mathsf{X} = \mathbb{R}^d$ or $\mathsf{X} = \mathbb{T}^d$ where $\mathbb{T} = \mathbb{R}/\mathbb{Z}$. Assume that π has a density with respect to the Lebesgue measure also denoted π and of the form $\pi = \mathrm{e}^{-U} / \int_{\mathbb{R}^d} \mathrm{e}^{-U(y)} \mathrm{d}y$ where $U \colon \mathsf{X} \to \mathbb{R}$ is a continuously differentiable function and is referred to as the potential associated with π. Sampling from such distributions is of interest in computational statistical mechanics and in Bayesian statistics and allows one, for example, to compute efficiently expectations of functions $f : \mathsf{X} \to \mathbb{R}$ with respect to π by invoking empirical process limit theorems, e.g. the law of large numbers. In practical set-ups, sampling exactly from π directly is either impossible or computationally prohibitive. A standard and versatile approach to sampling from such distributions consists of using Markov Chain Monte

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Carlo (MCMC) techniques [30, 41, 54], where the ability of simulating realizations of ergodic Markov chains leaving π invariant is exploited. Markov Process Monte Carlo (MPMC) methods are the continuous time counterparts of MCMC but their exact implementation is most often impossible on computers and requires additional approximation, such as time discretization of the process in the case of the Langevin diffusion. A notable exception, which has recently attracted significant attention, is the class of MPMC relying on Piecewise Deterministic Markov Processes (PDMP) [17], which in addition to being simpler to simulate than earlier MPMC, are nonreversible, offering the promise of better performance. We now briefly introduce a class of processes covering existing algorithms. The generic mathematical notation we use in the introduction is fairly standard and fully defined at the end of the section.

Known PDMP Monte Carlo methods rely on the use of the auxiliary variable trick, that is the introduction of an instrumental variable and probability distribution μ defined on an extended domain, of which π is a marginal distribution, which may facilitate simulation. In the present set-up, one introduces the velocity variable $v \in \mathsf{V} \subset \mathbb{R}^d$ associated with a probability distribution ν defined on the σ-field $\mathcal{V}$ of V, where the subset V is assumed to be closed. Standard choices for ν include the centered normal distribution with covariance matrix $m_2 \, \mathrm{I}_d$, where I_d is the d-dimensional identity matrix, the uniform distribution on the unit sphere $\mathbb{S}^{d-1}$, or the uniform distribution on $\mathsf{V} = \{-1, 1\}^d$. Let $\mathsf{E} = \mathsf{X} \times \mathsf{V}$ and define the probability measure $\mu = \pi \otimes \nu$. The aim is now to sample from the probability distribution μ.

We denote by $\mathrm{C}^2_{\mathrm{b}}(\mathsf{E})$ the set of bounded functions of $\mathrm{C}^2(\mathsf{E})$. The PDMP Monte Carlo algorithms we are aware of fall in a class of processes associated with generators of the form, for $f \in \mathrm{C}^2_{\mathrm{b}}(\mathsf{E})$ and $(x, v) \in \mathsf{E}$,

$$\mathcal{L}_1 f(x,v) = v^\top \nabla_x f(x,v) + \sum_{k=1}^{K} \lambda_k(x,v) \left(\mathcal{B}_k - \mathrm{Id}\right) f(x,v) + m_2^{1/2} \lambda_{\mathrm{ref}}(x) \mathcal{R}_v f(x,v) \;, \tag{1}$$

where $K \in \mathbb{N}$, $\lambda_k : \mathsf{E} \to \mathbb{R}_+$ for $k \in \{1, \ldots, K\}$, $\lambda_{\mathrm{ref}} : \mathsf{X} \to \mathbb{R}_+$, $(\mathcal{R}_v, \mathrm{D}(\mathcal{R}_v))$ and $(\mathcal{B}_k, \mathrm{D}(\mathcal{B}_k))$ for $k \in \{1, \ldots, K\}$ are operators we specify below, and

$$m_2 = \int_{\mathsf{V}} v_1^2 \, \mathrm{d}\nu(v) \;, \tag{2}$$

which is assumed to be finite. For any $k \in \{1, \ldots, K\}$, λ_k will be referred to as a jump rate and λ_{ref} as the refreshment rate.

In the case where $\mathsf{V} = \mathbb{R}^d$ and ν is the zero-mean Gaussian distribution on $\mathbb{R}^d$ with covariance matrix $m_2 \, \mathrm{I}_d$, we also consider generators of the form, for any $f \in \mathrm{C}^2_{\mathrm{b}}(\mathsf{E})$ and $(x, v) \in \mathsf{E}$,

$$\mathcal{L}_2 f(x,v) = \mathcal{L}_1 f(x,v) - m_2 F_0(x)^\top \nabla_v f(x,v) \;, \tag{3}$$

where $F_0 : \mathsf{X} \to \mathbb{R}^d$.

For any $k \in \{1, \ldots, K\}$, the jump operators $\mathcal{B}_k$ we consider are associated with continuous vector fields $F_k : \mathsf{X} \to \mathbb{R}^d$ of the form, for any $f : \mathsf{E} \to \mathbb{R}$ and $(x, v) \in \mathsf{E}$,

$$\mathcal{B}_k f(x,v) = f\left(x, v - 2\big(v^\top \mathrm{n}_k(x)\big)\, \mathrm{n}_k(x)\right) \;, \quad \mathrm{n}_k(x) = \begin{cases} F_k(x)/\left|F_k(x)\right| & \text{if } F_k(x) \neq 0 \;, \\ 0 & \text{otherwise} \;. \end{cases} \tag{4}$$

These operators correspond to reflections of the velocity through the hyperplanes orthogonal to $F_k(X)$ at the event position X, *i.e.* a flip of the component of the velocity in the direction given by F_k inducing an elastic "bounce" of the position trajectory with the hyperplane. As we shall see, the $K+1$ vector fields F_k are tied to the potential U by the relation $\nabla_x U = \sum_{k=0}^{K} F_k$, required to ensure that μ is left invariant by the associated semi-group. Informally, assuming for the moment that $\lambda_{\mathrm{ref}} = 0$ and $F_0 = \nabla_x U_0$ for some $U_0 \colon \mathsf{X} \to \mathbb{R}$, the corresponding process follows the solution of Hamilton's equations $(\dot{x}_t, \dot{v}_t) = \big(v_t, -\nabla_x U_0(x_t)\big)$ for a random time of distribution governed by an inhomogeneous Poisson process with rate $(x,v) \mapsto \sum_{k=1}^{K} \lambda_k(x,v)$. When an event occurs and the current state of the process is (X,V), one chooses between the K possible updates of the state available, with probability proportional to $\lambda_1(X,V), \ldots, \lambda_K(X,V)$, with the particularity here that the position X is left unchanged.

The vector fields $\{F_k : \mathsf{X} \to \mathbb{R}^d \, ; \, k \in \{1,\ldots,K\}\}$ and jump rates $\{\lambda_k : \mathsf{E} \to \mathbb{R}_+ \, ; \, k \in \{1,\ldots,K\}\}$ are linked by the relations $\lambda_k(x,v) - \lambda_k(x,-v) = v^\top F_k(x)$ for $k \in \{1,\ldots,K\}$ and $(x,v) \in \mathsf{E}$, together with other conditions, required to ensure that μ is an invariant distribution of the associated semi-group. A standard choice, sometimes referred to as canonical, consists of choosing jump rates $\lambda_k(x,v) = [v^\top F_k(x)]_+$ for $k \in \{1,\ldots,K\}$ and $(x,v) \in \mathsf{E}$.

Denote by $\mathrm{L}^2(\mu)$ the set of measurable functions $g : \mathsf{E} \to \mathbb{R}$ such that $\int_{\mathsf{E}} g^2 \, \mathrm{d}\mu < +\infty$. We let $\|\cdot\|_2$ be the norm induced by the scalar product

$$\text{for all } f, g \in \mathrm{L}^2(\mu) \, , \quad \langle f, g \rangle_2 = \int_{\mathsf{E}} f \, g \, \mathrm{d}\mu \, , \tag{5}$$

making $\mathrm{L}^2(\mu)$ a Hilbert space.

The operator $\mathcal{R}_v$ will be referred to as the refreshment operator, a standard example of which is $\mathcal{R}_v = \Pi_v - \mathrm{Id}$ where Π_v is the following orthogonal projector in $\mathrm{L}^2(\mu)$: for any $f \in \mathrm{L}^2(\mu)$,

$$\Pi_v f(x,v) = \int_{\mathsf{V}} f(x,w) \, \mathrm{d}\nu(w) \, , \tag{6}$$

in which case the velocity is drawn afresh from the marginal invariant distribution, while the position is left unchanged. In this scenario the informal description of the process given above carries on with $\lambda_{\mathrm{ref}} \neq 0$ added to the rate $(x,v) \mapsto \sum_{k=1}^{K} \lambda_k(x,v)$, Π_v an additional possible update to the velocity chosen with probability proportional to λ_{ref}. Another possible choice is the generator of an Ornstein-Uhlenbeck operator leaving ν invariant.

In all the paper we assume the following condition to hold for either $\mathcal{L}_1$ or $\mathcal{L}_2$, a condition satisfied by the examples covered in this manuscript.

A1. *(a) The operator $\mathcal{L}$ is closed in $\mathrm{L}^2(\mu)$, generates a strongly continuous contraction semi-group $(P_t)_{t \geq 0}$ on $\mathrm{L}^2(\mu)$, i.e. $P_0 = \mathrm{Id}$, for any $t, s \in \mathbb{R}_+$, $P_{s+t} = P_s P_t$, for any $f \in \mathrm{L}^2(\mu)$, $\|P_t f\|_2 \leq \|f\|_2$ and $\lim_{t \to 0} \|P_t f - f\|_2 = 0$.*

(b) μ is a a stationary measure for $(P_t)_{t \geq 0}$, i.e. for any $t \in \mathbb{R}_+$, $\mu P_t = \mu$.

(c) There exists a core C for $\mathcal{L}$ such that C is dense in $\mathrm{L}^2(\mu)$ and $\mathsf{C} \subset \mathrm{D}(\mathcal{L}) \cap \mathrm{D}(\mathcal{L}^\star)$, where $(\mathcal{L}^\star, \mathrm{D}(\mathcal{L}^\star))$ is the adjoint of $\mathcal{L}$ on $\mathrm{L}^2(\mu)$.

Note that if $\mathcal{L}$ generates a strongly continuous contraction semi-group then $\mathrm{D}(\mathcal{L})$ is dense by [27, Theorem 2.12] and the adjoint of $\mathcal{L}$ on $\mathrm{L}^2(\mu)$ is therefore well-defined and closed by [49, Theorem 5.1.5], and $\mathrm{D}(\mathcal{L}^\star)$ is dense.

We now describe how various choices of K and F_k lead to known algorithms. For simplicity of exposition, we assume for the moment that $\mathsf{V} = \mathbb{R}^d$, ν is the zero-mean Gaussian distribution with covariance matrix $m_2 \, \mathrm{I}_d$ and $\mathcal{R}_v = \Pi_v - \mathrm{Id}$, but as we shall see later our results cover more general scenarios.

- The particular choice $K = 0$ and $F_0 = \nabla_x U$ corresponds to the procedure described in [23] as a motivation for the popular hybrid Monte Carlo method. This process is also known as the Linear Boltzman/kinetic equation in the statistical physics literature [5] or randomized Hamiltonian Monte Carlo [11]. In this scenario the process follows the isocontours of μ for random times distributed according to an inhomogeneous Poisson law of parameter $\lambda_{\mathrm{ref}} > 0$, triggering events where the velocity is sampled afresh from ν.
- The scenario where $K = d$, $F_0 = 0$ and for $k \in \{1, \ldots, d\}$, $x \in \mathsf{X}$, $F_k(x) = \partial_k U(x)\mathbf{e}_k$ where $(\mathbf{e}_k)_{k\in\{1,\ldots,d\}}$ is the canonical basis, corresponds to the Zig-Zag (ZZ) process [6], where the x component of the process follows straight lines in the direction v which remains constant between events. In this scenario, the choice of $\mathcal{B}_k$ to update the velocity, consists of negating its k-th component; see also [29] for related ideas motivated by other applications.
- The standard Bouncy Particle Sampler (BPS) of [51], extended by [12], correspond to the choice $K = 1$, $F_0 = 0$ and $F_1 = \nabla_x U$.
- More elaborate versions of the ZZ and BPS processes, motivated by computational considerations, take advantage of the possibility to decompose the energy as $U = \sum_{k=0}^{K} U_k$ and corresponds to the choice $F_k = \nabla_x U_k$ [43, 12], where in the former the sign flip operation is replaced with a component swap.
- It should be clear that one can consider more general deterministic dynamics with $F_0 \neq 0$, effectively covering the Hamiltonian Bouncy Particle Sampler, suggested in [55].
- We remark that the well-known Langevin algorithm corresponds to $K = 0$, $F_0 = \nabla_x U$ and the situation where $\mathcal{R}_v$ is the Ornstein-Uhlenbeck process.

More general bounces involving randomization (see [55, 58, 44]) can also be considered in our framework, at the cost of additional complexity and reduced tightness of our bounds.

The main aim of the present paper is the study of the long time behaviour for the class of processes described above using hypercoercivity methods popularized by [57]. More precisely, consider $(P_t)_{t\geq 0}$ the semigroup associated to the PDMP with generator $\mathcal{L} \in \{\mathcal{L}_1, \mathcal{L}_2\}$ defined above, we aim to find simple and verifiable conditions on $U, F_k, \mathcal{R}_v$ and λ_{ref} ensuring the existence of $A \geq 1$ and $\alpha > 0$, and their explicit computation in terms of characteristics of the data of the problem, such that for any $f \in \mathrm{L}^2_0(\mu) := \left\{ g \in \mathrm{L}^2(\mu) : \int_{\mathsf{E}} g \, \mathrm{d}\mu = 0 \right\}$ and $t \geq 0$,

$$\|P_t f\|_2 \leq A \mathrm{e}^{-\alpha t} \|f\|_2 \ . \tag{7}$$

Establishing such a result is of interest to practitioners for multiple reasons. Explicit bounds may provide insights into expected performance properties of the algorithm in various situations or regimes. In particular the above leads to an upper bound on the integrated autocorrelation, which is a performance measure of Monte Carlo estimators of $\int_{\mathsf{E}} f \, \mathrm{d}\mu$, $f \in \mathrm{L}^2_0(\mu)$, defined by

$$\lim_{T\to\infty} T \, \mathrm{Var}_\mu \left(T^{-1} \int_0^T f(X_t, V_t) \, \mathrm{d}t \right) / \, \|f\|^2_{\mathrm{L}^2(\pi)} \leq 2A/\alpha \ ,$$

where $(X_t, V_t)_{t\geq 0}$ is a trajectory of a PDMP process of generator $\mathcal{L}$ with (X_0, V_0) distributed according to μ. For a class of problems of, say, increasing dimension $d \to \infty$, weak dependence of A and α on d indicates scalability of the method. It is worth pointing out that the result above is equivalent to the existence of $A \geq 1$ and $\alpha > 0$ such that for any measure $\rho_0 \ll \mu$ such that $\|\mathrm{d}\rho_0/\mathrm{d}\mu\|_2 < \infty$

$$\|\rho_0 P_t - \mu\|_{\mathrm{TV}} = \int_{\mathsf{E}} |\mathrm{d}(\rho_0 P_t)/\mathrm{d}\mu - 1| \, \mathrm{d}\mu \leq \|\mathrm{d}(\rho_0 P_t)/\mathrm{d}\mu - 1\|_{\mathrm{L}^2(\pi)} \leq A\mathrm{e}^{-\alpha t} \|\mathrm{d}\rho_0/\mathrm{d}\mu - 1\|_{\mathrm{L}^2(\pi)} \ ,$$

where the leftmost inequality is standard and a consequence of the Cauchy-Schwarz inequality. Our hypocoercivity result therefore also allows characterization of convergence to equilibrium of PDMPs in various scenarios and regimes, leading in particular to the possibility to compare performance of algorithms started from the same initial distribution. Establishing similar results for different metrics may be a useful complement to our characterization of algorithmic computational complexity and is left for future work.

In [46, 57], convergence of the type (7) is established using an appropriate H^1-norm associated with μ. The method which was developed in these papers is closely related to hypoellipticity theory [39, 26, 37] for Partial Differential Equation and in particular the kinetic Fokker-Planck equation. Convergence for linear Boltzman equations was first derived in [36, 46]. Since then, several works have extended and completed these results [21, 35, 1, 14, 28, 45].

Notation and conventions

The canonical basis of $\mathbb{R}^d$ is denoted by $(\mathbf{e}_i)_{i\in\{1,\ldots,d\}}$ and the d-dimensional identity matrix I_d. The Euclidean norm on $\mathbb{R}^d$ or $\mathbb{R}^{d\times d}$ is denoted by $|\cdot|$, and is associated with the usual Frobenius inner product $\mathrm{Tr}(\Phi^\top\Gamma)$ for any Φ, Γ in $\mathbb{R}^d$ or $\mathbb{R}^{d\times d}$.

Let M be a smooth submanifold of $\mathbb{R}^n$, for $n \in \mathbb{N}$. For any $k \in \mathbb{N}$, denote by $\mathrm{C}^k(\mathsf{M}, \mathbb{R}^m)$ the set of k-times differentiable functions from M to $\mathbb{R}^m$, $\mathrm{C}^k_{\mathrm{b}}(\mathsf{M}, \mathbb{R}^m)$ stands for the subset of bounded functions in $\mathrm{C}^k(\mathsf{M}, \mathbb{R}^m)$ with bounded differentials up to order k. $\mathrm{C}^k(\mathsf{M})$ and $\mathrm{C}^k_{\mathrm{b}}(\mathsf{M})$ stand for $\mathrm{C}^k(\mathsf{M}, \mathbb{R})$ and $\mathrm{C}^k_{\mathrm{b}}(\mathsf{M}, \mathbb{R})$ respectively.

For $f : \mathsf{X} \to \mathbb{R}$ and $i \in \{1, \ldots, d\}$, $x \mapsto \partial_{x_i} f(x)$ stands for the partial derivative of f with respect to the i^{th}-coordinate, if it exists. Similarly, for $f : \mathsf{X} \to \mathbb{R}$, $i, j \in \{1, \ldots, d\}$, denote by $\partial_{x_i,x_j} f = \partial_{x_i}\partial_{x_j} f$ when $\partial_{x_i}\partial_{x_j} f$ exists. For $f = (f_1, \ldots, f_m) \in \mathrm{C}^1(\mathsf{X}, \mathbb{R}^m)$, $\nabla_x f$ stands for the gradient of f defined for any $x \in \mathsf{X}$ by $\nabla_x f(x) = (\partial_{x_j} f_i(x))_{i\in\{1,\ldots,m\},\, j\in\{1,\ldots,d\}} \in \mathbb{R}^{d\times m}$. For ease of notation, we also denote by $(\nabla_x, \mathrm{D}(\nabla_x))$ the densely defined closed extension of $(\nabla_x, \mathrm{C}^1_{\mathrm{b}}(\mathsf{X}))$ on $\mathrm{L}^2(\pi)$, see [40, p. 88]. For any $f \in \mathrm{C}^k(\mathsf{X}, \mathbb{R}^m)$, $k \in \mathbb{N}$ and $p \geq 0$, define

$$\|f\|_{k,p} = \sup_{x\in\mathsf{X}} \sup_{(i_1,\ldots,i_k)\in\{1,\ldots,d\}^k} \left\{ \|\partial_{x_{i_1},\ldots,x_{i_k}} f(x)\| / (1 + \|x\|^p) \right\} \ .$$

We set for $k \geq 0$,

$$\mathrm{C}^k_{\mathrm{poly}}(\mathsf{X}, \mathbb{R}^m) = \left\{ f \in \mathrm{C}^k(\mathsf{X}, \mathbb{R}^m) \ : \ \inf_{p\geq 0} \|f\|_{k,p} < +\infty \right\} ,$$

and $\mathrm{C}^k_{\mathrm{poly}}(\mathsf{X})$ simply stands for $\mathrm{C}^k_{\mathrm{poly}}(\mathsf{X}, \mathbb{R})$. For any $f \in \mathrm{C}^2(\mathsf{X}, \mathbb{R})$, we let $\Delta_x f$ denote the Laplacian of f. Id stands for the identity operator. For two self-adjoint operators $(\mathcal{A}, \mathrm{D}(\mathcal{A}))$ and $(\mathcal{B}, \mathrm{D}(\mathcal{B}))$ on a Hilbert space H equipped with the scalar product $\langle\cdot,\cdot\rangle$ and norm $\|\cdot\|$, denote by $\mathcal{A} \succeq \mathcal{B}$ if

$\langle f, \mathcal{A}f\rangle \geq \langle f, \mathcal{B}f\rangle$ for all $f \in \mathrm{D}(\mathcal{A}) \cap \mathrm{D}(\mathcal{B})$. Then, define $(\mathcal{AB}, \mathrm{D}(\mathcal{AB}))$ with domain, if not specified, $\mathrm{D}(\mathcal{AB}) = \mathrm{D}(\mathcal{B}) \cap \{\mathcal{B}^{-1}\mathrm{D}(\mathcal{A})\}$. For a bounded operator $\mathcal{A}$ on H, we let $|||\mathcal{A}||| = \sup_{f\in\mathsf{H}} \|\mathcal{A}f\|/\|f\|$. Π is said to be an orthogonal projection if Π is a bounded symmetric operator H and $\Pi^2 = \Pi$. An unbounded operator $(\mathcal{A}, \mathrm{D}(\mathcal{A}))$ is said to be symmetric (respectively anti-symmetric) is for any $f, g \in \mathrm{D}(\mathcal{A})$, $\langle \mathcal{A}f, g\rangle = \langle f, \mathcal{A}g\rangle$ (respectively $\langle \mathcal{A}f, g\rangle = -\langle f, \mathcal{A}g\rangle$). If $\mathcal{A}$ is densily defined, $\mathcal{A}$ is said to be self-adjoint if $\mathcal{A} = \mathcal{A}^\star$. If in addition $\mathcal{A}$ is closed, $\mathsf{C} \subset \mathrm{D}(\mathcal{A})$ is said to be a core for $\mathcal{A}$ if the closure of $\mathcal{A}_{|\mathsf{C}}$ is $\mathcal{A}$. Denote by 1_F the constant function equals to 1 from a set F to $\mathbb{R}$. For any unbounded operator $(\mathcal{A}, \mathrm{D}(\mathcal{A}))$, we denote by $\mathrm{Ran}(\mathcal{A}) = \{\mathcal{A}f : f \in \mathrm{D}(\mathcal{A})\}$ and $\mathrm{Ker}(\mathcal{A}) = \{f \in \mathrm{D}(\mathcal{A}) : \mathcal{A}f = 0\}$. For any probability measure m on a measurable space $(\mathsf{M}, \mathcal{F})$, we denote by $\mathrm{L}^2(\mathrm{m})$ the Hilbert space of measurable functions f satisfying $\int_\mathsf{M} f^2 \mathrm{dm} < +\infty$, equipped with the inner product $\langle f, g\rangle_\mathrm{m} = \int_\mathsf{M} fg\, \mathrm{dm}$, and $\mathrm{L}^2_0(\mathrm{m}) = \{f \in \mathrm{L}^2(\mathrm{m}) : \int_\mathsf{M} f \mathrm{dm} = 0\}$. We will use the same notation for vector and matrix fields $\Phi, \Gamma \in (\mathbb{R}^d)^\mathsf{M}$ or $(\mathbb{R}^{d\times d})^\mathsf{M}$, *i.e.* $\langle \Phi, \Gamma\rangle_\mathrm{m} = \int_\mathsf{M} \mathrm{Tr}\left(\Phi^\top \Gamma\right) \mathrm{dm}$ and no confusion should be possible. When $m = \mu$ we replace m with 2 in this notation. For any $x \in \mathsf{M}$ denote by δ_x the Dirac distribution at x. We define the total variation distance between two probability measures $\mathrm{m}_1, \mathrm{m}_2$ on $(\mathsf{M}, \mathcal{F})$ by $\|\mathrm{m}_1 - \mathrm{m}_2\|_{\mathrm{TV}} = \sup_{\mathsf{A}\in\mathcal{F}} |\mathrm{m}_1(\mathsf{A}) - \mathrm{m}_2(\mathsf{A})|$. For a square matrix A we let $\mathrm{diag}(A)$ be its main diagonal and for a vector $v \in \mathbb{R}^d$ we let $\mathrm{diag}(v)$ be the square matrix of diagonal v and with zeros elsewhere. For $a, b \in \mathbb{R}$ we let $a \wedge b$ denote their minimum. For $a, b \in \mathbb{R}^d$ ($A, B \in \mathbb{R}^{d\times d}$), we denote by $a \odot b \in \mathbb{R}^d$ ($A \odot B \in \mathbb{R}^{d\times d}$) the Hadamard product between a and b defined for any $i \in \{1, \ldots, d\}$ ($i, j \in \{1, \ldots, d\}$) by $(a \odot b)_i = a_i b_i$ ($(A \odot B)_{i,j} = A_{i,j} B_{i,j}$). For any $i, j \in \mathbb{N}$, $\delta_{i,j}$ denotes the Kronecker symbol which is 1 if $i = j$ and 0 otherwise. For any $n_1, n_2 \in \mathbb{N}$, $n_1 < n_2$, we let $\sum_{n_2}^{n_1} = 0$.

2 Main results and organization of the paper

We now state our main results. In the following, for any densely defined operator $(\mathcal{C}, \mathrm{D}(\mathcal{C}))$ we let $(\mathcal{C}^\star, \mathrm{D}(\mathcal{C}^\star))$ denote its $\mathrm{L}^2(\mu)$-adjoint. First we specify conditions imposed on the potential U.

H1. *The potential* $U \in \mathrm{C}^3_{\mathrm{poly}}(\mathsf{X})$ *and satisfies*

(a) there exists $c_1 \geq 0$ *such that, for any* $x \in \mathsf{X}$, $\nabla^2_x U(x) \succeq -c_1 \mathrm{I}_d$*;*

(b)

$$\liminf_{|x|\to\infty} \left\{|\nabla_x U(x)|^2/2 - \Delta_x U(x)\right\} > 0 \,.$$

From [50, 3], **H**1-(b) is equivalent to assuming that π satisfies a Poincaré inequality on X, that is the existence of $C_\mathrm{P} > 0$ such that, for any $f \in \mathrm{C}^2(\mathsf{X})$ satisfying $\int_\mathsf{X} f \mathrm{d}\pi = 0$,

$$\|\nabla_x f\|_2^2 \geq C_\mathrm{P} \|f\|_2^2 \,. \tag{8}$$

Further, **H**1-(b) also implies the existence of $c_2 > 0$ and $\varpi \geq 0$ such that for any $x \in \mathsf{X}$,

$$\Delta_x U(x) \leq c_2 d^{1+\varpi} + |\nabla_x U(x)|^2/2 \,. \tag{9}$$

H 1-(b) indeed implies that the quantity considered is bounded from below, the scaling in d in front of c_2 will appear natural in the sequel. We have opted for this formulation of the assumption required of the potential to favour intuition and link it to the necessary and sufficient condition for geometric convergence of Langevin diffusions, but our quantitative bounds below will be given in terms of the Poincaré constant C_{P} for simplicity (see [4, Section 4.2] for quantitative estimates of C_{P} depending on potentially further conditions on U). **H**1-(a) is realistic in most applications, can be checked in practice and has the advantage of leading to simplified developments. It is possible to replace this assumption with $\sup_{x\in\mathsf{X}}\{|\nabla_x^2 U(x)|/(1+|\nabla_x U(x)|)\}<\infty$ and rephrase our results in terms of any finite upper bound of this quantity (see [21, Sections 2 and 3]). Finally the Poincaré inequality (8) implies by [4, Proposition 4.4.2] that there exists $s>0$ such that

$$\int_{\mathbb{R}^d} \mathrm{e}^{s|x|}\,\mathrm{d}\pi(x) < +\infty\,. \tag{10}$$

H2. *The family of vector fields* $\{F_k : \mathsf{X}\to\mathbb{R}^d\,;\, k\in\{0,\ldots,K\}\}$ *satisfies*

(a) for $k\in\{0,\ldots,K\}$, $F_k\in \mathrm{C}^2(\mathsf{X},\mathbb{R}^d)$;

(b) for all $x\in\mathsf{X}$, $\nabla_x U(x)=\sum_{k=0}^K F_k(x)$;

(c) for all $k\in\{0,\ldots,K\}$ *there exists* $a_k\geq 0$ *such that for all* $x\in\mathsf{X}$,

$$|F_k|(x)\leq a_k\left\{1+|\nabla_x U|(x)\right\}\,. \tag{11}$$

This assumption is in particular trivially true for the Zig-Zag and the Bouncy Particle Samplers. In turn we assume the jump rates to be related to the family of vector fields $\{F_k:\mathsf{X}\to\mathbb{R}^d\,;\,k\in\{1,\ldots,K\}\}$ through the following conditions.

H3. *There exist a continuous function* $\varphi:\mathbb{R}\to\mathbb{R}_+$, $C_\varphi\geq 1$ *and* $c_\varphi\geq 0$ *satisfying for any* $s\in\mathbb{R}$,

$$\varphi(s)-\varphi(-s)=s\,,\qquad \text{and}\qquad |s|\leq\varphi(s)+\varphi(-s)\leq c_\varphi m_2^{1/2}+C_\varphi\,|s|\,, \tag{12}$$

such that for any $k\in\{1,\ldots,K\}$ *and* $(x,v)\in\mathsf{E}$, $\lambda_k(x,v)=\varphi\big(v^\top F_k(x)\big)$.

We note that the canonical choice $\varphi(s)=(s)_+$ satisfies these conditions and that the first condition of (12) is equivalent to $\varphi(s)-(s)_+=\varphi(-s)-(-s)_+$, implying that $\varphi(s)\geq(s)_+$ for all $s\in\mathbb{R}$ and therefore that the left hand side inequality in (12) is automatically satisfied. If we further assume the existence of $C,c\geq 0$ such that for all $s\in\mathbb{R}$, $\varphi(s)\leq cm_2^{1/2}+C\,(s)_+$ then the second inequality is satisfied with $C_\varphi=C$ and $c_\varphi=2c$. As remarked in [2], the first condition of (12) holds for rates based on the choice

$$\varphi(s):=-\log\left(\phi\big(\exp(-s)\big)\right),$$

such that $\phi\colon\mathbb{R}_+\to[0,1]$ satisfies $r\phi(r^{-1})=\phi(r)$ for all $r\in\mathbb{R}_+\setminus\{0\}$. The canonical choice corresponds to $\phi(r)=1\wedge r$, but the (smooth) choice $\phi(r)=r/(1+r)$ is also possible.

H4. *Assume that* V *and* ν *satisfy the following conditions.*

(a) V *is stable under bounces, i.e. for all* $(x,v)\in\mathsf{E}$ *and* $k\in\{1,\ldots,K\}$, $v-2(v^\top\mathrm{n}_k(x))\,\mathrm{n}_k(x)\in\mathsf{V}$, *where* $\mathrm{n}_k(x)$ *is defined by* (4).

(b) For any $\mathsf{A}\in\mathcal{V}$, $x\in\mathsf{X}$, *we have* $\nu\left(\left\{\mathrm{Id}-2\mathrm{n}_k(x)\mathrm{n}_k(x)^\top\right\}\mathsf{A}\right)=\nu(\mathsf{A})$, *for any* $k\in\{1,\ldots,K\}$.

(c) For any bounded and measurable function $g:\mathbb{R}^2\to\mathbb{R}$, $i,j\in\{1,\ldots,d\}$ *such that* $i\neq j$, $\int_{\mathsf{V}} g(v_i,v_j)\,\mathrm{d}\nu(v)=\int_{\mathsf{V}} g(-v_1,v_2)\,\mathrm{d}\nu(v)$;

(d) ν has finite fourth order marginal moment

$$m_4 = (1/3)\left\|v_1^2\right\|_2^2 = (1/3)\int_{\mathsf{V}} v_1^4 \,\mathrm{d}\nu(v) < +\infty ,$$

and for any $i,j,k,l \in \{1,\ldots,d\}$ such that $\mathrm{card}(\{i,j,k,l\}) > 2$, $\int_{\mathsf{V}} v_i v_j v_k v_l \,\mathrm{d}\nu(v) = 0$.

Note that in the case where V and ν are rotation invariant, *i.e.* for any rotation O on $\mathbb{R}^d$, $O\mathsf{V} = \mathsf{V}$ and for any $\mathsf{A} \in \mathcal{V}$, $\nu(O\mathsf{A}) = \nu(\mathsf{A})$, then **H**4-(a)-(b)-(c) are automatically satisfied.

By **H**4-(c), we have $\int_{\mathsf{V}} v_1 v_2 \mathrm{d}\nu(x) = 0$ taking $g(v_1,v_2) = v_1 v_2$ for any $(v_1,v_2) \in \mathbb{R}^2$ and therefore for any $i,j \in \{1,\ldots,d\}$ such that $i \neq j$, $\int_{\mathsf{V}} v_i v_j \,\mathrm{d}\nu(v) = 0$. In addition, under **H**4-(d), from the Cauchy-Schwarz inequality, we obtain that

$$m_{2,2} = \|v_1 v_2\|_2^2 = \int_{\mathsf{V}} v_1^2 v_2^2 \,\mathrm{d}\nu(v) < \infty ,$$

and note that in the Gaussian case we have the relation $m_4 = m_{2,2} = m_2^2$. Finally, under **H**4, for any $f,g \in \mathrm{L}^2(\mu)$ and $k \in \{1,\ldots,K\}$, $\langle \mathcal{B}_k f, g\rangle_2 = \langle f, \mathcal{B}_k g\rangle_2$, that is $\mathcal{B}_k$ is symmetric on $\mathrm{L}^2(\mu)$.

In this paper we consider operators $(\mathcal{R}_v, \mathrm{D}(\mathcal{R}_v))$ on $\mathrm{L}^2(\mu)$ satisfying the following conditions.

H5. *(a) Functions depending only on the position belong to the kernel of $\mathcal{R}_v$:* $\mathrm{L}^2(\pi) \subset \mathrm{D}(\mathcal{R}_v)$ *and for any $f \in \mathrm{L}^2(\pi)$, $\mathcal{R}_v f = 0$;*

(b) $\mathcal{R}_v$ satisfies the detailed balance condition: $\mathcal{R}_v = \mathcal{R}_v^\star$ and $\mathrm{C}^2_{\mathrm{poly}}(\mathsf{E}) \subset \mathrm{D}(\mathcal{R}_v)$;

(c) $\mathcal{R}_v$ admits a spectral gap of size 1 on $\mathrm{L}^2_0(\nu)$: for any $g \in \mathrm{L}^2_0(\nu) \cap \mathrm{D}(\mathcal{R}_v)$, $\langle -\mathcal{R}_v g, g\rangle_2 \geq \|g\|_2^2$; in addition, for any $f \in \mathrm{L}^2(\pi)$, it holds for any $i \in \{1,\ldots,d\}$, $v_i f \in \mathrm{D}(\mathcal{R}_v)$ and $-\mathcal{R}_v(v_i f) = v_i f$.

Typically, $\mathcal{R}_v$ is of the form $\mathrm{Id} \otimes \tilde{\mathcal{R}}_v$ where $(\tilde{\mathcal{R}}_v, \mathrm{D}(\tilde{\mathcal{R}}_v))$ is a self-adjoint operator on $\mathrm{L}^2(\nu)$ with spectral gap equals 1. Then, condition **H**5-(a) is equivalent to $\tilde{\mathcal{R}}_v(1_{\mathsf{V}}) = 0$, which implies that for any $g \in \mathrm{D}(\tilde{\mathcal{R}}_v)$, we have

$$\int_{\mathsf{V}} \mathcal{R}_v g \,\mathrm{d}\nu = \langle 1_{\mathsf{E}}, \mathcal{R}_v g\rangle_2 = \langle \mathcal{R}_v^\star(1_{\mathsf{V}}), g\rangle_2 = \langle \mathcal{R}_v(1_{\mathsf{V}}), g\rangle_2 = 0 ,$$

so that the process associated with $\tilde{\mathcal{R}}_v$ preserves the probability measure ν.

Note that **H**5-(a) implies that $\mathcal{R}_v \Pi_v = 0$, whereas **H**5-(c) implies that $-\mathcal{R}_v(v_1 \Pi_v) = v_1 \Pi_v$, where Π_v is defined by (6). Assumption **H**5 is satisfied when $\mathcal{R}_v = \Pi_v$, or $\mathcal{R}_v = \mathrm{Id} \otimes \tilde{\mathcal{R}}_v$ with $\tilde{\mathcal{R}}_v$ the generator of the Ornstein-Uhlenbeck process defined for any $g \in \mathrm{C}^2_{\mathrm{b}}(\mathbb{R}^d)$ by

$$\tilde{\mathcal{R}}_v g = -\nabla_v g^\top v + \Delta_v g .$$

H6. *The refreshment rate $\lambda_{\mathrm{ref}} : \mathsf{X} \to \mathbb{R}_+$ is bounded from below and from above as follows: there exist $\underline{\lambda} > 0$ and $c_\lambda \geq 0$ such that for all $x \in \mathsf{X}$,*

$$0 < \underline{\lambda} \leq \lambda_{\mathrm{ref}}(x) \leq \underline{\lambda}(1 + c_\lambda |\nabla_x U(x)|) .$$

Under the previous assumptions we can prove exponential convergence of the semigroup.

Theorem 1. *Assume that $\mathcal{L}_i$, $i \in \{1,2\}$ given by (1) or (3) satisfies* **A** *1 with* $\mathsf{C} = \mathrm{C}^2_{\mathrm{b}}(\mathsf{E})$ *and* **H***1,* **H***2,* **H***3,* **H***4,* **H***5 and* **H***6 hold. Then there exist $A > 0$ and $\alpha > 0$ such that, for any $f \in \mathrm{L}^2_0(\mu)$, and $t \in \mathbb{R}_+$,*

$$\|P_t f\|_2 \leq A\,\mathrm{e}^{-\alpha t}\,\|f\|_2 \ .$$

The constants A and α are given in explicit form in (20) in Theorem 4 (Section 3), in terms of the constant appearing in **H***1,* **H***2,* **H***4,* **H***5 and* **H***6, where ϵ can be taken to be ϵ_0 given in (22), $\lambda_v = \underline{\lambda}$, $\lambda_x = C_{\mathrm{P}}/(1 + C_{\mathrm{P}})$ and $R_0 = (4 + 2\sqrt{3}) \vee (\underline{\lambda}/2^{1/2}) \vee \overline{R}_0$ where*

$$\overline{R}_0 = \frac{\sqrt{2m_{2,2} + 3(m_4 - m_{2,2})_+}}{m_2}\left\{\frac{2^{1/2}(1+C_\varphi)\kappa_1}{\kappa_2}\sum_{k=1}^{K} a_k + \kappa_1\right\} + \frac{\underline{\lambda}}{2^{1/2}}\left\{1 + \frac{2c_\lambda\kappa_1}{\kappa_2}\right\} + \frac{c_\varphi K}{2^{1/2}} \ , \quad (13)$$

$$\kappa_1 = (1 + c_1/2)^{1/2} \ \text{and} \ \kappa_2^{-1} = C_{\mathrm{P}}^{-1}(1 + 4c_2 d^{1+\varpi} + 16C_{\mathrm{P}}^2)^{1/2}.$$

Proof. The proof is postponed to Section 4.1. □

The following details the expected scaling behaviour with d of A and α. The proof can be found in Section 4.3.

Corollary 2. *Consider the assumptions and notation of Theorem 1. Further suppose that there exists $m_b > 0$ satisfying*

$$m_2^{-1}\sqrt{2m_{2,2} + 3(m_4 - m_{2,2})_+} \leq m_b \ , \quad (14)$$

which together with C_{P}, c_1, c_2 and $\|a\|_\infty = \sup_{k\in\{1,\dots,K\}} a_k$ are independent of d. Then $A \leq 3^{1/2}$ and there exists $C^\alpha(C_{\mathrm{P}}, c_1, c_2, \|a\|_\infty, m_b) > 0$, independent of $d, \underline{\lambda}, c_\lambda$ and C_φ, c_φ, such that for d large enough,

$$\alpha > C^\alpha(C_{\mathrm{P}}, c_1, c_2, \|a\|_\infty, m_b)\,\underline{\lambda}\,m_2^{1/2}\left[\{c_\varphi K\} \vee \{(1+C_\varphi)d^{(1+\varpi)/2}K + 1\} \vee \{\underline{\lambda}(1 + c_\lambda d^{(1+\varpi)/2})\}\right]^{-2} . \quad (15)$$

Thus, if $\underline{\lambda}$, c_λ, C_φ and c_φ are fixed, we get that α^{-1} is in general at most of order $\mathcal{O}(m_2^{-1/2} d^{1+\varpi} K^2)$ if $K \geq 1$.

We now discuss the assumptions of the theorem, and application of its conclusion to various instances of PDMP-MC and two examples of potentials. Assumption **H**1 is problem dependent and verifiable in practice, while **H**2, **H**4, **H**5 and **H**6 are user controllable and we have already discussed standard choices satisfying these conditions. More delicate may be establishing that **A** 1 holds and that $\mathrm{C}^2_{\mathrm{b}}(\mathsf{E})$ is indeed a core for the generator $\mathcal{L}$. As shown in [25], BPS and ZZ are well defined Markov process whose generators admit $\mathrm{C}^2_{\mathrm{b}}(\mathsf{E})$ as a core and similar arguments can be used to establish that it is also a core for the RHMC. Further, it is not difficult to show that for the class of processes described earlier, for any $f \in \mathrm{C}^2_{\mathrm{b}}(\mathsf{E})$, $\langle \mathcal{L}f, \mathbf{1}\rangle_2 = 0$, therefore implying that μ is an invariant distribution and that **A**1 holds.

First we note that the spectral gap is indeed expected to be proportional to $m_2^{1/2}$, since if $(X_t, V_t)_{t\geq 0}$ is a PDMP with generator of the form (1) or (3) for $m_2 = 1$, then $(X_{m^{1/2}t}, m^{1/2}V_{m^{1/2}t})_{t\geq 0}$ is a PDMP with generator of the same form with $m_2 = m$. We therefore set $m_2 = 1$ below, a condition satisfied when ν is the uniform distribution on the sphere $\sqrt{d}\,\mathbb{S}^{d-1}$or $\{-1,1\}^d$, or the d-dimensional zero-mean Gaussian distribution with covariance matrix I_d, all of which also satisfy (14). More generally, by Lemma 36 in Appendix D, property (14) is satisfied if ν is a spherically symmetric distribution on $\mathbb{R}^d$ corresponding to random variables $V = B^{1/2}W$ for W uniformly

<table>
<tr><th></th><th>$\underline{\lambda}$</th><th>α</th><th>$U(x) = \sum_{i=1}^{d}(1+x_i^2)^{\beta}/2$</th><th>$U(x) = (1+\lvert x\rvert^2)^{\beta}$</th></tr>
<tr><td>RHMC</td><td>$\Theta(1)$</td><td>$\omega\big(\underline{\lambda}\wedge\underline{\lambda}^{-1}\big)$</td><td rowspan="3">$\beta \geq 1\,, \quad \varpi = 0$</td><td rowspan="3">$\beta \geq 1\,, \quad \varpi = 1 - 1/\beta$</td></tr>
<tr><td>BPS</td><td>$\Theta\big(d^{(1+\varpi)/2}\big)$</td><td>$\omega\big(d^{-(1+\varpi)/2}\big)$</td></tr>
<tr><td>ZZ (crude)</td><td>$\Theta\big(d^{(3+\varpi)/2}\big)$</td><td>$\omega\big(d^{-(3+\varpi)/2}\big)$</td></tr>
<tr><td>ZZ (Section 5)</td><td>$\Theta(1)$</td><td>$\omega(1)$</td><td>$\beta \geq 1$</td><td>$\beta = 2$</td></tr>
</table>

Table 1: Left hand side: summary of the dependence of α on d for $C_P, c_1, c_2, \|a\|_\infty$ constant, $m_2 = 1$ and optimal choice of $\underline{\lambda}$. Right hand side: summary of application to two examples of potentials.

distributed on the hypersphere $\sqrt{d}\,\mathbb{S}^{d-1}$ and B a non-negative random variable independent of W and of first and second order moments γ_1 and γ_2 respectively such that $\gamma_2^{1/2}/\gamma_1$ is upper bounded by a constant independent of the dimension.

By [4, Proposition 5.1.3, Corollary 5.7.2], independence of C_P on d is satisfied for strongly convex potentials U: *i.e.* whenever there exists $m > 0$ such that $\nabla_x^2 U(x) \succeq m\,\mathrm{I}_d$ for any $x \in \mathbb{R}^d$ which implies that one can take $C_\mathrm{P} = m$. This is the case for $U(x) = \sum_{i=1}^{d}\big(1+x_i^2\big)^{\beta}/2$ or $U(x) = (1+|x|^2)^{\beta}$ with $\beta \geq 1$, for which (9) is also satisfied with $\varpi = 0$ and $\varpi = 1 - 1/\beta$ respectively (see Lemma 40 and Lemma 41 in Appendix F). We note that from the Holley-Stroock perturbation principle [38], uniformly bounded perturbations of a strongly convex potential lead to independence of C_P on d. For $\beta \in [1/2, 1)$ $C_\mathrm{P} > 0$, but is dependent on d, see [4, Chapter 4]. However recent progress in the precise quantitative estimation of spectral gaps of certain probability measures [9, 10] allows for the strong convexity property to be relaxed to simple convexity and beyond, but leads to a dependence of C_P on d which can be characterised.

Now further assume that C_φ, c_φ and that the refreshment rate are uniformly bounded in the position x, implying $c_\lambda = 0$. Then by Corollary 2-(15), there exists $C^\alpha(C_\mathrm{P}, c_1, c_2, \|a\|_\infty, m_b, c_\varphi, C_\varphi) > 0$ such that for d sufficiently large

$$\alpha \geq C^\alpha(C_\mathrm{P}, c_1, c_2, \|a\|_\infty, m_b, c_\varphi, C_\varphi)\,\left\{\left[\underline{\lambda}\big(1 + K^2 d^{1+\varpi}\big)^{-1/2}\right] \wedge \underline{\lambda}^{-1}\right\}\,,$$

from which we deduce the optimal scaling of the refreshment rate, namely $C_1^{\underline{\lambda}}\big(1 + K^2 d^{1+\varpi}\big)^{1/2} \leq \underline{\lambda} \leq C_2^{\underline{\lambda}}\big(1 + K^2 d^{1+\varpi}\big)^{1/2}$ for $C_1^{\underline{\lambda}}, C_2^{\underline{\lambda}} > 0$ (which we denote $\Theta\big((1 + K^2 d^{1+\varpi})^{1/2}\big)$ hereafter to alleviate notation). Using the description of RHMC, ZZ and BPS provided in the introduction we deduce the first three lines of Table 1, where $\alpha = \omega(s)$ is used as a short hand notation for $\alpha \geq C^\alpha(C_\mathrm{P}, c_1, c_2, \|a\|_\infty, m_b, c_\varphi, C_\varphi)s$ for $s \to 0$. The fourth line uses our specialised results of Section 5, showing that the conclusion of Theorem 2 is not optimal for ZZ.

In [7] scaling limits of particular functionals of the ZZ and BPS processes are studied, leading to quantitative estimates of the time required to achieve near independence at equilibrium. More specifically they consider the scenario where the target distribution is a centred normal distribution of covariance matrix I_d and focus on the angular momentum, the negative log-target density and the first coordinate of the process. Our more general results, obtained using a different argument, are in agreement after noticing that [7] considered the scenario $m_2 = d^{-1}$ and using our earlier remark on the dependence of our estimate of the absolute spectral gap on $m_2^{1/2}$. In [19] it is shown, again using an approach different from ours, that the RHMC has dimension free convergence rate in a scenario similar to ours.

While nonreversibily of the processes considered here may be practically beneficial, it is only recently that the tools allowing our work have been developed [56, 57]. Our method of proof relies on the framework proposed recently in [20, 21, 13] to study the solutions of the forward Kolmogorov equation associated with the linear kinetic process, but we study the dual backward Kolmogorov equation for a broader class of processes as is the case in [31, 32, 33] who provide the first rigorous derivation of the results of [20, 21, 13]. This, combined with the flexibility of the framework of [21, 13] explains the differing inner product used throughout, which we have found to lead to simpler computations while yielding identical conclusions. The estimate (7) (with constant $A = 1$) would follow straightforwardly from a Grönwall argument if the generator $\mathcal{L}$ of the semigroup was coercive, that is it satisfied $\langle \mathcal{L}f, f \rangle_2 \leq -a \|f\|_2^2$ for some $a > 0$ and any f in a core of $\mathcal{L}$. Unfortunately, the symmetric part of the generator corresponding to a PDMP is degenerate in general, in the sense that it has a nontrivial null space. Hence, the aforementioned coercivity clearly fails to hold. However, it is possible to equip $\mathrm{L}^2(\mu)$ with an equivalent scalar product derived from $\langle \cdot, \cdot \rangle_2$ with respect to which $\mathcal{L}$ is coercive. The constant α is then given by the coercivity bound, while the constant A can be obtained from estimates relating the two equivalent scalar products.

The paper is organised as follows. In Section 3 we develop our framework for hypocoercivity suited to PDMP-MC processes, based on the ideas of [21]. In addition to providing a rigorous framework we further optimize the constants involved, ultimately leading to Theorem 1. The proofs of Theorem 1 and its corollary are given in Section 4. In Section 5, we specialize our results to the case of the Zig-Zag process for which better estimates are possible, leading to attractive scaling properties with the dimension d. Various intermediate technical results have been moved to Appendices where, for completeness, we have also included classical facts from functional analysis.

3 The DMS framework for hypocoercivity

As stated above our results rely on the ideas proposed by [20, 21, 13] for which a rigorous framework was subsequently given in [31, 32, 33, 34]. We derive here a novel proof, which borrows elements of [31, 32, 33, 34] but leads to a different set of conditions motivated by our application to PDMP-Monte Carlo methods. We further provide explicit and optimized estimates of the constants involved in terms of accessible characteristics of the process. We first present abstract results which form the core of all of our proofs and then establish more specific ones common to all the processes considered in this paper, implying some of the abstract conditions. More specific results relating to the Zig-Zag process are treated in Section 5.

3.1 Abstract DMS results

We let $\mathcal{S}$ and $\mathcal{T}$ be the $\mathrm{L}^2(\mu)$-symmetric and $\mathrm{L}^2(\mu)$-anti-symmetric parts of a generator $\mathcal{L}$ satisfying **A**1, that is

$$\mathcal{S} = (\mathcal{L} + \mathcal{L}^\star)/2 \quad \text{and} \quad \mathcal{T} = (\mathcal{L} - \mathcal{L}^\star)/2 \,, \quad \text{defined on } \mathrm{D}(\mathcal{S}) = \mathrm{D}(\mathcal{T}) = \mathsf{C} \,. \tag{16}$$

Consider the following additional assumption to **A**1.

A2. $\Pi_v \mathsf{C} \subset \mathsf{C}$ *and* $(\mathcal{T}\Pi_v, \mathsf{C})$ *is a closable operator, where* Π_v *is defined by* (6) *and* C *is given in* ***A*** *1.*

Note that since $\Pi_v \mathsf{C} \subset \mathsf{C}$, we have $\mathsf{C} \subset \mathrm{D}(\mathcal{T}\Pi_v)$ and the restriction of $\mathcal{T}\Pi_v$ to C exists. Under **A**1 and **A**2, Lemma 28 in Appendix B justifies the definition of the operator $\mathcal{A}$,

$$\mathcal{A} = \left(m_2 \,\mathrm{Id} + (\mathcal{T}\Pi_v)^\star (\overline{\mathcal{T}\Pi_v})\right)^{-1} (-\mathcal{T}\Pi_v)^\star \,, \quad \mathrm{D}(\mathcal{A}) = \mathrm{D}((\mathcal{T}\Pi_v)^\star) \,, \tag{17}$$

where m_2 is given by (2) and $(\overline{\mathcal{T}\Pi_v}, \mathrm{D}(\overline{\mathcal{T}\Pi_v}))$ and $((\mathcal{T}\Pi_v)^\star, \mathrm{D}((\mathcal{T}\Pi_v)^\star))$ are the closure and the adjoint of $(\mathcal{T}\Pi_v, \mathsf{C})$ respectively. Key properties are that $\mathrm{Ran}(\mathcal{A}) \subset \mathrm{D}(\overline{\mathcal{T}\Pi_v})$, $\mathcal{A}$ is closable with $\overline{\mathcal{A}}$ bounded, and $\overline{\mathcal{T}\Pi_v}\mathcal{A}$ is also closable of bounded closure. To show this result we adapt [31, Lemma 2.4] since their lemma assumes that $(\mathcal{T}, \mathrm{D}(\mathcal{T}))$ is closed whereas, motivated by our applications, we assume $(\mathcal{T}\Pi_v, \mathsf{C})$ to be a densely defined and closable operator instead.

Lemma 3. *Let $(\mathcal{T}, \mathrm{D}(\mathcal{T}))$ be a anti-symmetric densely defined operator on $\mathrm{L}^2(\mu)$. Assume that there exists $\mathsf{D} \subset \mathrm{D}(\mathcal{T}\Pi_v) \cap \mathrm{D}(\mathcal{T})$, such that $(\mathcal{T}\Pi_v, \mathsf{D})$ is a densely defined closable operator.*

(a) The closure of $(\mathcal{T}\Pi_v, \mathsf{D})$, $(\overline{\mathcal{T}\Pi_v}, \mathrm{D}(\overline{\mathcal{T}\Pi_v}))$ satisfies $\mathrm{D}(\overline{\mathcal{T}\Pi_v}) \subset \mathrm{D}((\Pi_v\mathcal{T})^\star)$ and for any $f \in \mathrm{D}(\overline{\mathcal{T}\Pi_v})$, $(\Pi_v\mathcal{T})^\star f = -\overline{\mathcal{T}\Pi_v} f$, where $((\mathcal{T}\Pi_v)^\star, \mathrm{D}((\mathcal{T}\Pi_v)^\star))$ is the adjoint of $(\mathcal{T}\Pi_v, \mathsf{D})$.

(b) The operator $\mathcal{A}$ defined by (17) satisfies $\mathrm{Ran}(\mathcal{A}) \subset \mathrm{D}(\overline{\mathcal{T}\Pi_v})$, is closable and its closure $\overline{\mathcal{A}}$ is a bounded operator on $\mathrm{L}^2(\mu)$ with $\|\overline{\mathcal{A}}\|_2 \leq 1/(2m_2)^{1/2}$ and $\Pi_v\overline{\mathcal{A}} = \overline{\mathcal{A}}$ on $\mathrm{L}^2(\mu)$.

(c) Assume in addition that for any $f \in \mathsf{D}$, $\Pi_v\mathcal{T}\Pi_v f = 0$. Then, $(\overline{\mathcal{T}\Pi_v}\mathcal{A}, \mathrm{D}(\overline{\mathcal{T}\Pi_v}\mathcal{A}))$ is also closable and its closure $\mathcal{E}$ is bounded and satisfies for any $f \in \mathrm{L}^2(\mu)$, $\|\mathcal{E}f\|_2 \leq \|(\mathrm{Id} - \Pi_v)f\|_2$.

Proof. To establish this result, we make use of classical results on unbounded operators in Hilbert spaces which for completeness, are given in Appendix B.

(a) Since $\mathcal{T}$ is assumed to be anti-symmetric, we have for any $f \in \mathrm{D}(\mathcal{T}\Pi_v)$, $g \in \mathsf{D}$, $\langle \Pi_v\mathcal{T}f, g\rangle_2 = -\langle f, \mathcal{T}\Pi_v g\rangle_2$ since $\Pi_v g \in \mathrm{D}(\mathcal{T})$ as $\mathsf{D} \subset \mathrm{D}(\mathcal{T}\Pi_v)$. By definition of $(\mathcal{T}\Pi_v)^\star$, we obtain that $\mathsf{D} \subset \mathrm{D}((\Pi_v\mathcal{T})^\star)$, and for any $f \in \mathsf{D}$, $\mathcal{T}\Pi_v f = -(\Pi_v\mathcal{T})^\star f$. Therefore $\{(f, \mathcal{T}\Pi_v f) : f \in \mathsf{D}\} \subset \{(f, -(\Pi_v\mathcal{T})^\star f) : f \in \mathrm{D}((\Pi_v\mathcal{T})^\star)\}$, and we obtain the desired result by definition of $(\overline{\mathcal{T}\Pi_v}, \mathrm{D}(\overline{\mathcal{T}\Pi_v}))$ since $-(\Pi_v\mathcal{T})^\star$ is closed by [49, Theorem 5.1.5].

(b) The fact that $\mathrm{Ran}(\mathcal{A}) \subset \mathrm{D}(\overline{\mathcal{T}\Pi_v})$, $\mathcal{A}$ is closable and the bound follow directly from Lemma 28 and Proposition 26-(a)-(d). We turn to the statement $\Pi_v\overline{\mathcal{A}} = \overline{\mathcal{A}}$. By Lemma 28, the operator $\mathcal{C} = (m_2 \mathrm{Id} + (\mathcal{T}\Pi_v)^\star(\overline{\mathcal{T}\Pi_v}))^{-1}$ is well-defined, bounded and $\mathrm{Ran}(\mathcal{C}) = \mathrm{D}((\mathcal{T}\Pi_v)^\star(\overline{\mathcal{T}\Pi_v}))$. Therefore using Lemma 30-(a) (since $\mathcal{T}\Pi_v$ is densely defined), we have for any $f \in \mathrm{D}(\mathcal{T})$,

$$\mathcal{A}f = \mathcal{C}\Pi_v\mathcal{T}f = m_2^{-1}\left\{\mathrm{Id} - (\mathcal{T}\Pi_v)^\star(\overline{\mathcal{T}\Pi_v})\mathcal{C}\right\}\Pi_v\mathcal{T}f \; . \tag{18}$$

Therefore, by applying Π_v to both sides and using Lemma 30-(b), we deduce that for any $f \in \mathrm{D}(\mathcal{T})$, $\Pi_v\mathcal{A}f = \mathcal{A}f$. The proof is then concluded upon noting that $\mathrm{D}(\mathcal{T})$ is dense and Π_v is continuous.

(c) For any $f \in \mathsf{D}$, since $\Pi_v\mathcal{T}\Pi_v f = 0$, (18) becomes

$$\mathcal{A}f = \mathcal{C}\Pi_v\mathcal{T}(\mathrm{Id} - \Pi_v)f = m_2^{-1}\left\{\mathrm{Id} - (\mathcal{T}\Pi_v)^\star(\overline{\mathcal{T}\Pi_v})\mathcal{C}\right\}\Pi_v\mathcal{T}(\mathrm{Id} - \Pi_v)f \; .$$

Therefore, we get for any $f \in \mathsf{D}$,

$$\begin{aligned}
\|\mathcal{A}f\|_2^2 &= m_2^{-1}\left\{\langle \Pi_v\mathcal{T}(\mathrm{Id} - \Pi_v)f, \mathcal{A}f\rangle_2 - \left\langle (\mathcal{T}\Pi_v)^\star(\overline{\mathcal{T}\Pi_v})\mathcal{C}\Pi_v\mathcal{T}(\mathrm{Id} - \Pi_v)f, \mathcal{A}f\right\rangle_2\right\} \\
&= m_2^{-1}\left\{\langle -(\mathcal{T}\Pi_v)^\star(\mathrm{Id} - \Pi_v)f, \mathcal{A}f\rangle_2 - \left\langle (\mathcal{T}\Pi_v)^\star(\overline{\mathcal{T}\Pi_v})\mathcal{C}\Pi_v\mathcal{T}(\mathrm{Id} - \Pi_v)f, \mathcal{A}f\right\rangle_2\right\} \\
&= m_2^{-1}\left\{-\left\langle (\mathrm{Id} - \Pi_v)f, (\overline{\mathcal{T}\Pi_v})\mathcal{A}f\right\rangle_2 - \left\|(\overline{\mathcal{T}\Pi_v})\mathcal{A}f\right\|_2^2\right\} \; ,
\end{aligned}$$

using successively that $(\mathrm{Id} - \Pi_v)f \in \mathrm{D}(\mathcal{T})$ since $f \in \mathsf{D} \subset \mathrm{D}(\mathcal{T}\Pi_v)$, Lemma 30 and $\mathcal{A}f \in \mathrm{D}(\overline{\mathcal{T}\Pi_v})$. Using the Cauchy-Schwarz inequality we obtain that for any $f \in \mathsf{D}$, $\|(\overline{\mathcal{T}\Pi_v})\mathcal{A}f\|_2 \leq \|(\mathrm{Id} - \Pi_v)f\|_2$. Using that D is dense in $\mathrm{L}^2(\mu)$ together with the bounded linear transformation extension theorem [53, Theorem I.7] concludes the proof.

□

The main result of [21] can be formulated under the following abstract assumption, which we shall assume to hold from now on, and the proof of our main theorem relies on optimized estimates of the constants involved.

A 3 (DMS abstract conditions)**.** *Let* C *be as in* ***A** 1. Assume further that it satisfies* ***A** 2 and the following conditions*

(a) there exists $\lambda_v > 0$ *satisfying for any* $f \in \mathsf{C}$

$$- \langle \mathcal{S}f, f\rangle_2 \geq \lambda_v m_2^{1/2} \|(\mathrm{Id} - \Pi_v)f\|_2^2 \ ;$$

(b) there exists $\lambda_x \in (0,1)$ *satisfying for any* $f \in \mathsf{C}$

$$- \langle \overline{\mathcal{A}}\mathcal{T}\Pi_v f, f\rangle_2 \geq \lambda_x \|\Pi_v f\|_2^2 \ ; \tag{19}$$

(c) there exists $R_0 \geq 0$ *satisfying for any* $f \in \mathsf{C}$

$$\left|\langle \overline{\mathcal{A}}\mathcal{T}(\mathrm{Id} - \Pi_v)f, f\rangle_2 + \langle \overline{\mathcal{A}}\mathcal{S}f, f\rangle_2\right| \leq R_0 \|(\mathrm{Id} - \Pi_v)f\|_2 \|\Pi_v f\|_2 \ ;$$

(d) for any $f \in \mathsf{C}$, $\Pi_v \mathcal{T} \Pi_v f = 0$*;*

(e) finally, $\mathrm{Ran}(\Pi_v) \subset \mathrm{Ker}(\mathcal{S}^\star)$.

Theorem 4. *Assume* ***A** 1,* ***A** 2 and* ***A** 3.*

(a) Then, for any $f \in \mathrm{L}^2_0(\mu)$, $t \in \mathbb{R}_+$ *and* $\epsilon \in (0, (2^{1/2}\lambda_v)^{-1} \wedge \{4\lambda_x/(4\lambda_x + R_0^2)\})$

$$\|P_t f\|_2 \leq A(\epsilon)\mathrm{e}^{-\alpha(\epsilon)t} \|f\|_2 \ ,$$

with

$$\alpha(\epsilon) = \lambda_v m_2^{1/2} \frac{\Lambda(\epsilon)}{1 + 2^{1/2}\lambda_v \epsilon} > 0 \quad \textit{and} \quad A(\epsilon) = \sqrt{\frac{1 + 2^{1/2}\lambda_v\epsilon}{1 - 2^{1/2}\lambda_v\epsilon}} \ , \tag{20}$$

where

$$\Lambda(\epsilon) = \frac{1 - \epsilon(1-\lambda_x) - \sqrt{[1 - \epsilon(1-\lambda_x)]^2 - 4\epsilon\lambda_x(1-\epsilon) + \epsilon^2 R_0^2}}{2} \ . \tag{21}$$

(b) Further, if $2^{1/2}R_0 \geq \lambda_v$ *then* $\alpha \colon \left(0, 4\lambda_x/(4\lambda_x + R_0^2)\right) \to \mathbb{R}_+$ *has a unique maximum at* $\epsilon^\star$ *such that* $\alpha(\epsilon_0) < \alpha(\epsilon^\star) < 3\alpha(\epsilon_0)$*, with*

$$\epsilon_0 = \frac{1 + \lambda_x - (1-\lambda_x)\sqrt{\frac{{R_0}^2}{{R_0}^2 + 4\lambda_x}}}{(1+\lambda_x)^2 + {R_0}^2} \in (0, (2^{1/2}\lambda_v)^{-1} \wedge \{4\lambda_x/(4\lambda_x + R_0^2)\}) \ , \tag{22}$$

so that $A(\epsilon_0) < +\infty$ *is well defined. In addition, if* $R_0 \geq 2$ *then* $\epsilon_0 < 3\lambda_x/(4\lambda_x + R_0^2)$.

The main idea of [21] behind the proof of Theorem 4 is the introduction of an equivalent norm for $\varepsilon \in \mathbb{R}_+$ (instead of the $\mathrm{L}^2(\mu)$ norm, which corresponds to $\varepsilon = 0$)

$$\mathscr{H}_\varepsilon(f) = (1/2) \|f\|_2^2 + \varepsilon \langle f, \overline{\mathcal{A}} f \rangle_2 ,$$

for which $(P_t)_{t\geq 0}$ is exponentially contracting. More precisely, [21, Theorem 2] shows that for some $\varepsilon \in (-(m_2/2)^{1/2}, (m_2/2)^{1/2})$ there exists $\alpha(\varepsilon) > 0$ such that for any $f \in \mathrm{L}_0^2(\mu)$, $\mathscr{H}_\varepsilon(P_t f) \leq \mathrm{e}^{-\alpha(\varepsilon)t} \mathscr{H}_\varepsilon(f)$. Then, the convergence in $\mathrm{L}_0^2(\mu)$ follows by Lemma 3-(b) which implies that $\mathscr{H}_\varepsilon(\cdot)$ defines a norm which is equivalent to $\|\cdot\|_2$: for $\varepsilon \in (-(m_2/2)^{1/2}, (m_2/2)^{1/2})$ and for any $f \in \mathrm{L}^2(\mu)$, it holds

$$(1 - (m_2/2)^{-1/2}\varepsilon) \|f\|_2^2 \leq 2\mathscr{H}_\varepsilon(f) \leq (1 + (m_2/2)^{-1/2}\varepsilon) \|f\|_2^2 . \tag{23}$$

Therefore, for a family $\{f_t \in \mathrm{L}^2(\mu)\}_{t\geq 0}$, exponential decay of $t \mapsto \mathscr{H}_\varepsilon(f_t)$ is equivalent to that of $t \mapsto \|f_t\|_2^2$, a property exploited in the following proof. We first establish the following results which give estimates of the functional $\{\mathscr{F}_i : i \in \{1, 2, 3\}\}$ defined for any $g \in \mathrm{D}(\mathcal{L})$ by

$$\mathscr{F}_1(g) = \langle \mathcal{L}g, g \rangle_2 \ , \quad \mathscr{F}_2(g) = \langle \mathcal{L}g, \overline{\mathcal{A}}g \rangle_2 \ , \quad \mathscr{F}_3(g) = \langle \overline{\mathcal{A}}\mathcal{L}g, g \rangle_2 \ . \tag{24}$$

Lemma 5. *Assume that $\mathcal{L}$ satisfies* **A***1,* **A***2, and* **A***3. Then, for any $g \in \mathrm{D}(\mathcal{L})$, we have*

$$\begin{aligned} \mathscr{F}_1(g) \leq -\lambda_v m_2^{1/2} \|(\mathrm{Id} - \Pi_v)g\|_2^2 \ , \quad \mathscr{F}_2(g) \leq \|(\mathrm{Id} - \Pi_v)g\|_2^2 \ , \\ \mathscr{F}_3(g) \leq -\lambda_x \|\Pi_v g\|_2^2 + R_0 \|(\mathrm{Id} - \Pi_v)g\|_2 \|\Pi_v g\|_2 \ . \end{aligned} \tag{25}$$

Proof. Note that since C is a core for $\mathcal{L}$ and $\overline{\mathcal{A}}$ and Π_v are bounded, we only need to show that (25) holds for all $g \in \mathsf{C}$. In addition, since $\overline{\mathcal{A}}$ is an extension of $\mathcal{A}$ by Lemma 3-(b), and for any $g \in \mathsf{C} \subset \mathrm{D}((\mathcal{T}\Pi_v)^\star) = \mathrm{D}(\mathcal{A})$ from Lemma 30-(a) as $\Pi_v(\mathsf{C}) \subset \mathsf{C} = \mathrm{D}(\mathcal{T})$ by **A**2, we deduce

$$\overline{\mathcal{A}}g = \mathcal{A}g \ . \tag{26}$$

Using that $\mathcal{S}$ is symmetric, $\mathcal{T}$ is anti-symmetric and $\mathsf{C} \subset \mathrm{D}(\mathcal{L}) \cap \mathrm{D}(\mathcal{L}^\star)$, we get that for any $g \in \mathsf{C}$, $\mathscr{F}_1(g) = \langle \mathcal{S}g, g \rangle_2 \leq -\lambda_v m_2^{1/2} \|(\mathrm{Id} - \Pi_v)g\|_2$ by **A**3-(a).

Second, using that $\Pi_v \overline{\mathcal{A}} = \overline{\mathcal{A}}$ by Lemma 3-(b) and (26), we have for any $g \in \mathsf{C}$,

$$\mathscr{F}_2(g) = \langle \Pi_v \mathcal{A}g, \mathcal{S}g \rangle_2 + \langle \Pi_v \mathcal{A}g, \mathcal{T}g \rangle_2 = \langle \Pi_v \mathcal{A}g, \mathcal{T}g \rangle_2 \ ,$$

where the last equality follows from $\mathrm{Ran}(\Pi_v) \subset \mathrm{Ker}(\mathcal{S}^\star)$. In addition, since Π_v is symmetric, $\Pi_v \mathcal{T} \Pi_v g = 0$, $\mathrm{Ran}(\mathcal{A}) \subset \mathrm{D}(\overline{\mathcal{T}\Pi_v}) \subset \mathrm{D}((\Pi_v \mathcal{T})^\star)$ by Lemma 3-(a)-(b), so $(\Pi_v \mathcal{T})^\star \mathcal{A} = -\overline{\mathcal{T}\Pi_v}\mathcal{A}$ by Lemma 3-(a) and $\|\overline{\mathcal{T}\Pi_v}\mathcal{A}g\|_2 \leq \|(\mathrm{Id} - \Pi_v)g\|_2$ by Lemma 3-(c), we obtain for any $g \in \mathsf{C}$,

$$\begin{aligned} \mathscr{F}_2(g) = \langle \mathcal{A}g, \Pi_v \mathcal{T}(\mathrm{Id} - \Pi_v)g \rangle_2 &= \langle (\Pi_v \mathcal{T})^\star \mathcal{A}g, (\mathrm{Id} - \Pi_v)g \rangle_2 \\ &= -\langle \overline{\mathcal{T}\Pi_v}\mathcal{A}g, (\mathrm{Id} - \Pi_v)g \rangle_2 \leq \|(\mathrm{Id} - \Pi_v)g\|_2^2 \ . \end{aligned}$$

Finally, using **A**3-(b)-(c) we have that for any $g \in \mathsf{C} \subset \mathrm{D}(\mathcal{L}) \cap \mathrm{D}(\mathcal{L}^\star) \cap \mathrm{D}(\mathcal{T}\Pi_v)$,

$$\mathscr{F}_3(g) = \langle \overline{\mathcal{A}}\mathcal{T}\Pi_v g, g \rangle_2 + \langle \overline{\mathcal{A}}\mathcal{T}(\mathrm{Id} - \Pi_v)g, g \rangle_2 + \langle \overline{\mathcal{A}}\mathcal{S}g, g \rangle_2 \leq -\lambda_x \|\Pi_v g\|_2^2 + R_0 \|(\mathrm{Id} - \Pi_v)g\|_2 \|\Pi_v g\|_2 \ .$$

□

Proof of Theorem 4. The first part of the proof follows along the same lines as [31, Theorem 2.18]. Let $f \in \mathrm{L}^2(\mu)$ satisfying $\int_{\mathsf{E}} f \mathrm{d}\mu = 0$ and $\varepsilon > 0$. For ease of notation, set for any $t \geq 0$, $f_t = P_t f$. From the Dynkin formula [27, Proposition 1.5], for any $t > 0$ $f_t \in \mathrm{D}(\mathcal{L})$ and $\mathrm{d}f_t/\mathrm{d}t = \mathcal{L} f_t$. Therefore, for any $t > 0$,

$$-\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{H}_\varepsilon(f_t) = -[\mathscr{F}_1(f_t) + \varepsilon\{\mathscr{F}_2(f_t) + \mathscr{F}_3(f_t)\}] ,$$

where $\{\mathscr{F}_i : i \in \{1,2,3\}\}$ are defined in (24). Then by Lemma 5, we obtain that for any $t > 0$,

$$\begin{aligned}
&-\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{H}_\varepsilon(f_t) \\
&\geq \lambda_v m_2^{1/2} \|(\mathrm{Id} - \Pi_v) f_t\|_2^2 + \varepsilon\left[\lambda_x \|\Pi_v f_t\|_2^2 - \|(\mathrm{Id} - \Pi_v) f_t\|_2^2 - R_0 \|(\mathrm{Id} - \Pi_v) f_t\|_2 \|\Pi_v f_t\|_2\right] \\
&= \begin{pmatrix} \|\Pi_v f_t\|_2 \\ \|(\mathrm{Id} - \Pi_v) f_t\|_2 \end{pmatrix}^\top \begin{pmatrix} \varepsilon\lambda_x & -\varepsilon R_0/2 \\ -\varepsilon R_0/2 & \lambda_v m_2^{1/2} - \varepsilon \end{pmatrix} \begin{pmatrix} \|\Pi_v f_t\|_2 \\ \|(\mathrm{Id} - \Pi_v) f_t\|_2 \end{pmatrix} \geq \Lambda_0(\varepsilon) \|f_t\|_2^2 ,
\end{aligned}$$

where

$$\Lambda_0(\varepsilon) = \frac{\lambda_v m_2^{1/2} - \varepsilon(1-\lambda_x) - \sqrt{(\lambda_v m_2^{1/2} - \varepsilon(1-\lambda_x))^2 - [4\varepsilon\lambda_x(\lambda_v m_2^{1/2} - \varepsilon) - \varepsilon^2 R_0^2]}}{2} ,$$

is the smallest eigenvalue of the symmetric matrix, positive for $0 \leq \varepsilon \leq 4\lambda_x\lambda_v m_2^{1/2}/(4\lambda_x + R_0^2)$ from Lemma 23 in Appendix A (as $\lambda_x \leq 1$ by **A**3-(b)). Using (23), we get

$$-\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{H}_\varepsilon(f_t) \geq \frac{2\Lambda_0(\varepsilon)}{1 + (m_2/2)^{-1/2}\varepsilon}\mathscr{H}_\varepsilon(f_t) .$$

From Grönwall's lemma and (23), we obtain for $0 \leq \varepsilon \leq (m_2/2)^{1/2} \wedge \{4\lambda_x\lambda_v m_2^{1/2}/(4\lambda_x + R_0^2)\}$,

$$\|f_t\|_2 \leq C_0(\varepsilon)\mathrm{e}^{-\alpha_0(\varepsilon)t}\|f_0\|_2 , \text{ where } \alpha_0(\varepsilon) = \frac{\Lambda_0(\varepsilon)}{1 + (m_2/2)^{-1/2}\varepsilon} \text{ and } C_0(\varepsilon) = \sqrt{\frac{1 + (m_2/2)^{-1/2}\varepsilon}{1 - (m_2/2)^{-1/2}\varepsilon}} .$$

For notational simplicity we let $\epsilon = \varepsilon/(\lambda_v m_2^{1/2})$ and note that with the definitions in (20)-(21), for $\epsilon < 4\lambda_x/(4\lambda_x + R_0^2)$, $\alpha(\epsilon) = \alpha_0(\varepsilon) > 0$ and $\lambda_v m_2^{1/2}\Lambda(\epsilon) = \Lambda_0(\varepsilon) > 0$, and for $\epsilon \leq (2^{1/2}\lambda_v)^{-1}$ the two norms are equivalent and $A(\epsilon) = A_0(\varepsilon)$ is well defined. This concludes the proof of (a).

From Proposition 25 and associated notation in Appendix A, $\epsilon \mapsto \alpha(\epsilon)$ has a unique, but intractable, maximum, $\epsilon^\star \in (0, 4\lambda_x/(4\lambda_x + R_0^2))$. However from Lemma 24-(b) and Proposition 25 the unique maximum $\epsilon_0 \in (\epsilon^\star, 4\lambda_x/(4\lambda_x + R_0^2))$ of $\epsilon \mapsto \Lambda(\epsilon)$, defined by (63), provides us with a tractable proxy such that $\alpha(\epsilon_0) < \alpha(\epsilon^\star) < 3\alpha(\epsilon_0)$. In addition, since $\lambda_x \leq 1$ and for $2^{1/2}R_0 \geq \lambda_v$ we get

$$\epsilon_0 < \frac{(1+\lambda_x)}{(1+\lambda_x)^2 + R_0^2} \leq (2R_0)^{-1} \leq (2^{1/2}\lambda_v)^{-1} ,$$

which implies that $A(\epsilon_0)$ is well defined (and the two norms equivalent). The last statement follows from Lemma 24-(c) in Appendix A.

□

The following lemma provides us with simple estimates of $\alpha(\epsilon_0)$ and $A(\epsilon_0)$ defined in Theorem 4.

Lemma 6. *Let $\epsilon \mapsto \alpha(\epsilon), A(\epsilon)$ and ϵ_0 be as in Theorem 4 and let $\lambda_x \in (0,1)$. Then*

(a) for any $R_0 \geq 4 + 12^{1/2}$,

$$\lambda_x/(1+R_0^2) \leq \epsilon_0 \leq 2/(4+R_0^2) \leq 1/(4R_0) \ , \tag{27}$$

(b) for any $R_0 \geq (4+12^{1/2}) \vee (\lambda_v/2^{1/2})$,

$$A(\epsilon_0) \leq 3^{1/2} \quad \text{and} \quad \lambda_v \lambda_x m_2^{1/2} \epsilon_0/6 \leq \alpha(\epsilon_0) \leq 4\lambda_v\lambda_x m_2^{1/2}\epsilon_0 \ .$$

Proof. The proof is postponed to Section 4.2. □

3.2 DMS for PDMP: generic results

Proposition 7. *Assume that $\mathcal{L}_i$, $i \in \{1,2\}$, defined by (1) or (3), with $\mathcal{B}_k$ given in (4), satisfies **A**1 with $\mathsf{C} = \mathrm{C}_\mathrm{b}^2(\mathsf{E})$ together with **H**1, **H**2, **H**3, **H**4 **H**5 and **H**6. Then the $\mathrm{L}^2(\mu)$-adjoint of $\mathcal{L}_i$ for $i \in \{1,2\}$ defined by (1) or (3) is given for any $f \in \mathrm{C}_\mathrm{b}^2(\mathsf{E})$ by*

$$\mathcal{L}_i^\star f = -v^\top \nabla_x f + \delta_{i,2} m_2 F_0^\top \nabla_v f + \sum_{k=1}^{K} \varphi\big(-v^\top F_k\big)[(\mathcal{B}_k - \mathrm{Id})f] + m_2^{1/2} \lambda_\mathrm{ref} \mathcal{R}_v f \ .$$

Proof. We only consider the case $i = 2$ since the proof for $i = 1$ follows along the same lines. In addition, since $\mathcal{R}_v$ is self-adjoint by **H**5 and $\mathrm{C}_\mathrm{b}^2(\mathsf{E}) \subset \mathrm{D}(\mathcal{R}_v)$, we can consider the case $\lambda_\mathrm{ref}(x) = 0$ for any $x \in \mathsf{X}$. Based on (1)-(3), using that for any $k \in \{1,\ldots,K\}$, $\mathcal{B}_k$ is symmetric on $\mathrm{L}^2(\mu)$, for any $(x,v) \in \mathsf{E}$, $\mathcal{B}_k\lambda_k(x,v) = \lambda_k(x,-v)$ and by integration by part, for any $f,g \in \mathrm{C}_\mathrm{b}^2(\mathsf{E})$, we obtain

$$\begin{aligned}
\langle g, \mathcal{L}f\rangle_2 &= \Big\langle -v^\top \nabla_x g + (v^\top \nabla_x U) g + m_2 F_0^\top \nabla_v g - (v^\top F_0) g + \textstyle\sum_{k=1}^K (\mathcal{B}_k - \mathrm{Id})[\lambda_k(x,v) g], f \Big\rangle_2 \\
&= \Big\langle -v^\top \nabla_x g + [v^\top (\nabla_x U - F_0)] g + m_2 F_0^\top \nabla_v g + \textstyle\sum_{k=1}^K \{\lambda_k(x,-v)\mathcal{B}_k g - \lambda_k(x,v) g\}, f \Big\rangle_2 \\
&= \langle \mathcal{L}_i^\star g, f\rangle_2 + \Big\langle [v^\top(\nabla_x U - F_0)] g + g \textstyle\sum_{k=1}^K \{\lambda_k(x,-v) - \lambda_k(x,v)\}, f \Big\rangle_2 \ .
\end{aligned}$$

Using that $\sum_{k=0}^K F_k = \nabla_x U$ by **H**2-(b) and that $\lambda_k(x,v) - \lambda_k(x,-v) = v^\top F_k(x)$ for any $k \in \{1,\ldots,K\}$ and $(x,v) \in \mathsf{E}$ by **H**3, concludes the proof.

□

The following provides expressions for the $\mathrm{L}^2(\mu)$-symmetric and $\mathrm{L}^2(\mu)$-anti-symmetric parts of $\mathcal{L}$ for all the PDMP processes considered in this paper. Define $\lambda_k^\mathrm{e} : \mathsf{E} \to \mathbb{R}_+$ for any $(x,v) \in \mathsf{E}$ and $k \in \{1,\ldots,K\}$ by

$$\lambda_k^\mathrm{e}(x,v) := \lambda_k(x,v) + \lambda_k(x,-v) \ . \tag{28}$$

Proposition 8. *Assume that $\mathcal{L}_i$, $i \in \{1,2\}$, defined by (1) or (3), with $\mathcal{B}_k$ given in (4), satisfies **A**1 with $\mathsf{C} = \mathrm{C}_\mathrm{b}^2(\mathsf{E})$ together with **H**1, **H**2, **H**3, **H**4 **H**5 and **H**6. Let $\mathcal{S}$ and $\mathcal{T}_i$ be the symmetric and anti-symmetric parts of $\mathcal{L}_i$ respectively, defined by (16).*

(a) Then for any $f \in \mathrm{C}_\mathrm{b}^2(\mathsf{E})$, $\mathcal{T}_i f = \tilde{\mathcal{T}}_i f$ and $\mathcal{S}_i f = \tilde{\mathcal{S}} f$ where $\tilde{\mathcal{T}}_i$ and $\tilde{\mathcal{S}}$ are the operators defined for any $g \in \mathrm{C}_\mathrm{poly}^2(\mathsf{E})$ by

$$\tilde{\mathcal{T}}_i g = v^\top \nabla_x g - \delta_{i,2} m_2 F_0^\top \nabla_v g + \frac{1}{2}\sum_{k=1}^{K} (v^\top F_k)\,(\mathcal{B}_k - \mathrm{Id})g \;, \tag{29}$$

$$\tilde{\mathcal{S}} g = \frac{1}{2}\sum_{k=1}^{K} \lambda_k^\mathrm{e}\,(\mathcal{B}_k - \mathrm{Id})g + m_2^{1/2} \lambda_\mathrm{ref} \mathcal{R}_v g \;. \tag{30}$$

*(b) $\mathcal{S}$ satisfies **A** 3-(e).*

(c) $\mathrm{C}_\mathrm{poly}^1(\mathsf{E}) \subset \mathrm{D}(\mathcal{T}_i^\star) \cap \mathrm{D}(\mathcal{S}^\star)$ and for any $f \in \mathrm{C}_\mathrm{poly}^1(\mathsf{E})$, $\mathcal{T}_i^\star f = -\tilde{\mathcal{T}}_i f$ and $\mathcal{S}^\star f = \tilde{\mathcal{S}} f$.

Note that the symmetric parts of $\mathcal{L}_i$ for $i \in \{1,2\}$ are the same and equal to $\mathcal{S}$.

Proof. (a) follows from Proposition 7 and the definitions of $\mathcal{S}$ and $\mathcal{T}$ in (16). (b) is a direct consequence of the first result and the definition of $(\mathcal{S}^\star, \mathrm{D}(\mathcal{S}^\star))$. Simple integration by parts and definitions of $(\mathcal{S}^\star, \mathrm{D}(\mathcal{S}^\star))$, $(\mathcal{T}_i^\star, \mathrm{D}(\mathcal{T}_i^\star))$ imply (c). □

We define the directional derivative operator

$$\text{for any } f \in \mathrm{D}(\mathcal{D}) = \mathrm{C}_\mathrm{b}^1(\mathsf{E}) \;,\; \mathcal{D}f(x,v) := v^\top \nabla_x f(x,v) \;. \tag{31}$$

The operators $(\mathcal{D}, \mathrm{C}_\mathrm{b}^1(\mathsf{E}))$ and $(\mathcal{D}\Pi_v, \mathrm{C}_\mathrm{b}^1(\mathsf{E}))$ are densely defined on $\mathrm{L}^2(\mu)$ and closable. The proof is similar to that for the operator ∇_x and is omitted, see for example [40, p. 88]. Note that by (29), a simple computation gives that for any $f \in \mathrm{C}_\mathrm{b}^2(\mathsf{E})$ and $i \in \{1,2\}$, since $\Pi_v f \in \mathrm{C}_\mathrm{b}^2(\mathsf{E})$,

$$\mathcal{T}_i \Pi_v f = \mathcal{D}\Pi_v f \;. \tag{32}$$

Lemma 9. *Assume that $\mathcal{L}_i$, $i \in \{1,2\}$, defined by (1) or (3), with $\mathcal{B}_k$ given in (4), satisfies **A** 1 with $\mathsf{C} = \mathrm{C}_\mathrm{b}^2(\mathsf{E})$ together with **H** 1, **H** 2, **H** 3, **H** 4 **H** 5 and **H** 6. Then, with $\mathcal{T}_i$ the anti-symmetric part of $\mathcal{L}_i$ defined by (16) and the operator $\mathcal{A}_i$ defined by (17) relative to $\mathcal{T}_i$, it holds:*

*(a) $\mathcal{T}_i$ satisfies **A** 2 and **A** 3-(d) with $\mathsf{C} = \mathrm{C}_\mathrm{b}^2(\mathsf{E})$ and $((\overline{\mathcal{T}_i \Pi_v}), \mathrm{D}(\overline{\mathcal{T}_i \Pi_v})) = ((\overline{\mathcal{D}\Pi_v}), \mathrm{D}(\overline{\mathcal{D}\Pi_v}))$;*

(b) $\mathrm{C}_\mathrm{b}^2(\mathsf{E}) \subset \mathrm{D}((\mathcal{T}_i \Pi_v)^\star \overline{\mathcal{T}_i \Pi_v})$ and for any $f \in \mathrm{C}_\mathrm{b}^2(\mathsf{E})$, $(\mathcal{T}_i \Pi_v)^\star \mathcal{T}_i \Pi_v f = m_2 \nabla_x^\star \nabla_x \Pi_v f$;

(c) $\{m_2 \mathrm{Id} + (\mathcal{T}_i \Pi_v)^\star \overline{\mathcal{T}_i \Pi_v}\}^{-1} \Pi_v = m_2^{-1} \{\mathrm{Id} + \nabla_x^\star \nabla_x\}^{-1} \Pi_v$ on $\mathrm{L}^2(\mu)$;

(d) $\mathcal{A}_i^\star = m_2^{-1} (\overline{\mathcal{D}\Pi_v}) \{\mathrm{Id} + \nabla_x^\star \nabla_x\}^{-1} \Pi_v$ and for any $f \in \mathrm{C}_\mathrm{b}^2(\mathsf{E})$, there exists a unique function $u \in \mathrm{C}_\mathrm{poly}^3(\mathsf{X})$, such that $m_2^{-1} \{\mathrm{Id} + \nabla_x^\star \nabla_x\}^{-1} \Pi_v f = u$ and

$$\mathcal{A}_i^\star f = -v^\top \nabla_x u = -m_2^{-1} (\overline{\mathcal{D}\Pi_v}) \{\mathrm{Id} + \nabla_x^\star \nabla_x\}^{-1} \Pi_v \;. \tag{33}$$

Proof. (a) First note that $\mathrm{C}_\mathrm{b}^2(\mathsf{E})$ is a core for $(\overline{\mathcal{D}\Pi_v}, \mathrm{D}(\overline{\mathcal{D}\Pi_v}))$ since for any $f \in \mathrm{C}_\mathrm{b}^1(\mathsf{E})$, there exists a sequence of functions $(f_n)_{n \in \mathbb{N}}$ such that for any $n \in \mathbb{N}$, $f_n \in \mathrm{C}_\mathrm{b}^2(\mathsf{E})$, $\lim_{n \to +\infty} \|f - f_n\|_2 = 0$ and $\lim_{n \to +\infty} \|\nabla_x f - \nabla_x f_n\|_2 = 0$. Then the proof is completed upon using (31) and (32).

(b) By (32), we have for any $f \in \mathrm{C}_\mathrm{b}^2(\mathsf{E})$, that $\mathcal{T}_i\Pi_v f = v^\top \nabla_x \Pi_v f$. It suffices then to verify that with $g : (x, v) \mapsto v^\top \nabla_x \Pi_v f(x, v)$, then $g \in \mathrm{D}((\mathcal{T}_i\Pi_v)^\star)$ and $(\mathcal{T}_i\Pi_v)^\star g = m_2 \nabla_x^\star g$, *i.e.* for any $h \in \mathrm{D}(\mathcal{T}_i\Pi_v)$, $\langle \mathcal{T}_i\Pi_v h, g\rangle_2 = m_2 \langle h, \nabla_x^\star g\rangle_2$. But $\mathrm{D}(\mathcal{T}_i\Pi_v) = \mathsf{C} = \mathrm{C}_\mathrm{b}^2(\mathsf{E})$ by assumption and definition see (16), and then the result is just a straightforward consequence of (31), (32) and an integration by part.

(c) Note that we only need to show that the two operators $\{m_2 \operatorname{Id} + (\mathcal{T}_i\Pi_v)^\star \overline{\mathcal{T}_i\Pi_v}\}^{-1}$ and $m_2^{-1}\{\operatorname{Id} + \nabla_x^\star \nabla_x\}^{-1}$ coincide on a dense subset of $\mathrm{L}^2(\pi)$ since they are bounded. We prove that this statement is true choosing the subset $m_2\{\operatorname{Id} + \nabla_x^\star\nabla_x\}(\mathrm{C}^3_\mathrm{poly}(\mathsf{X}))$. First, for any $h \in \mathrm{C}_\mathrm{b}^2(\mathsf{E})$, we have using (a), (b) and the definition (31) that

$$\{m_2 \operatorname{Id} + (\mathcal{T}_i\Pi_v)^\star \overline{\mathcal{T}_i\Pi_v}\}h = \{m_2 \operatorname{Id} + (\mathcal{T}_i\Pi_v)^\star \mathcal{T}_i\Pi_v\}h = m_2\{\operatorname{Id} + \nabla_x^\star \nabla_x \Pi_v\}h \; . \tag{34}$$

Second, for any $g \in \mathrm{C}^3_\mathrm{poly}(\mathsf{X})$, there exists a sequence $(g_n)_{n\in\mathbb{N}}$ such that for any $n \in \mathbb{N}$, $g_n \in \mathrm{C}_\mathrm{b}^2(\mathsf{X})$, $(g_n)_{n\in\mathbb{N}}$, $(\nabla_x g_n)_{n\in\mathbb{N}}$ and $(\nabla_x^2 g_n)_{n\in\mathbb{N}}$ converge in $\mathrm{L}^2(\pi)$ to g, $\nabla_x g$ and $\nabla_x^2 g$ respectively, which implies that $\{[m_2 \operatorname{Id} + (\mathcal{T}_i\Pi_v)^\star \overline{\mathcal{T}_i\Pi_v}]g_n\}_{n\in\mathbb{N}}$ and $\{m_2[\operatorname{Id} + (\nabla_x)^\star \nabla_x]g_n\}_{n\in\mathbb{N}}$ converge in $\mathrm{L}^2(\pi)$. Therefore, since $\{m_2 \operatorname{Id} + (\mathcal{T}_i\Pi_v)^\star \overline{\mathcal{T}_i\Pi_v}\}$ and $m_2\{\operatorname{Id} + \nabla_x^\star\nabla_x\}$ are closed, we get that $\mathrm{C}^3_\mathrm{poly}(\mathsf{X})$ is included in the domain of these two operators and (34) holds for any $h \in \mathrm{C}^3_\mathrm{poly}(\mathsf{X})$. [48, Theorem 2] or [15, Lemma 17][1] show that for any $f \in \mathrm{C}_\mathrm{b}^2(\mathsf{X})$, there exists $u \in \mathrm{C}^3_\mathrm{poly}(\mathsf{X})$ such that $m_2\{\operatorname{Id} + \nabla_x^\star\nabla_x\}u = f$. Therefore, it holds that $\mathrm{C}_\mathrm{b}^2(\mathsf{X}) \subset m_2\{\operatorname{Id} + \nabla_x^\star\nabla_x\}(\mathrm{C}^3_\mathrm{poly}(\mathsf{X}))$ so $m_2\{\operatorname{Id} + \nabla_x^\star\nabla_x\}(\mathrm{C}^3_\mathrm{poly}(\mathsf{X}))$ is dense in $\mathrm{L}^2(\pi)$. In addition, since we have shown that the operators $\{m_2 \operatorname{Id} + (\mathcal{T}_i\Pi_v)^\star \overline{\mathcal{T}_i\Pi_v}\}$ and $m_2\{\operatorname{Id} + \nabla_x^\star\nabla_x\}$ coincide on $\mathrm{C}^3_\mathrm{poly}(\mathsf{X})$, $\{m_2 \operatorname{Id} + (\mathcal{T}_i\Pi_v)^\star \overline{\mathcal{T}_i\Pi_v}\}^{-1}$ and $m_2^{-1}\{\operatorname{Id} + \nabla_x^\star\nabla_x\}^{-1}$ coincide on $m_2\{\operatorname{Id} + \nabla_x^\star\nabla_x\}(\mathrm{C}^3_\mathrm{poly}(\mathsf{X}))$.

(d) As $\mathcal{A}_i$ is bounded, it is sufficient to show that $\mathcal{A}_i^\star$ and $m_2^{-1}(\overline{\mathcal{D}\Pi_v})\{\operatorname{Id} + \nabla_x^\star\nabla_x\}^{-1}\Pi_v$ coincide on a dense subset of $\mathrm{L}^2(\mu)$. First, for all $f, g \in \mathrm{C}_\mathrm{b}^2(\mathsf{E})$, we get that $\langle \mathcal{A}_i g, f\rangle_2 = \langle \Pi_v \mathcal{A}_i g, f\rangle_2$ by Lemma 3-(b). Now using the definition of $\mathcal{A}_i$ (17), that Π_v and $\{m_2 \operatorname{Id} + (\mathcal{T}_i\Pi_v)^\star \overline{\mathcal{T}_i\Pi_v}\}^{-1}$ are bounded and self-adjoint, since Π_v is an orthogonal projection and by Proposition 26-(a)-(c), we get for any $f \in \mathrm{C}_\mathrm{b}^2(\mathsf{E})$,

$$\langle \mathcal{A}_i g, f\rangle_2 = m_2^{-1} \left\langle (-\Pi_v \mathcal{T}_i)^\star g, \{\operatorname{Id} + \nabla_x^\star\nabla_x\}^{-1}\Pi_v f\right\rangle_2 = m_2^{-1} \left\langle \mathcal{T}_i\Pi_v g, \{\operatorname{Id} + \nabla_x^\star\nabla_x\}^{-1}\Pi_v f\right\rangle_2 \; ,$$

where we have used Lemma 30-(a) for the last equality and $\mathrm{D}(\mathcal{T}) = \mathrm{C}_\mathrm{b}^2(\mathsf{E})$. [48, Theorem 2] or [15, Lemma 17] show that there exists $u \in \mathrm{C}^3_\mathrm{poly}(\mathsf{X})$ satisfying $m_2\{\operatorname{Id} + \nabla_x^\star\nabla_x\}u = \Pi_v f$ and therefore, we get that

$$\langle \mathcal{A}_i g, f\rangle_2 = \langle \mathcal{T}_i\Pi_v g, u\rangle_2 = -\left\langle g, v^\top \nabla_x u\right\rangle_2 \; ,$$

using an integration by part for the last identity. This result shows that for any $f \in \mathrm{C}_\mathrm{b}^2(\mathsf{E})$, we have that $\mathcal{A}_i^\star f = -v^\top\nabla_x u$. In addition, for any $g \in \mathrm{C}^1_\mathrm{poly}(\mathsf{E})$, there exists a sequence $(f_n)_{n\in\mathbb{N}}$ such that $f_n \in \mathrm{C}_\mathrm{b}^1(\mathsf{E})$ and $\lim_{n\to+\infty} \|g - f_n\|_2 = 0$, $\lim_{n\to+\infty} \|\nabla_x g - \nabla_x f_n\|_2 = 0$. Therefore we get that $\mathrm{C}^1_\mathrm{poly}(\mathsf{E}) \subset \mathrm{D}(\overline{\mathcal{D}\Pi_v})$ and for any $g \in \mathrm{C}^1_\mathrm{poly}(\mathsf{E})$, $\overline{\mathcal{D}\Pi_v} g(x, v) = v^\top\nabla_x g(x, v)$ for any $(x, v) \in \mathsf{E}$. Therefore, we get the desired conclusion that $\mathcal{A}_i^\star f = -v^\top\nabla_x u = -m_2^{-1}(\overline{\mathcal{D}\Pi_v})\{\operatorname{Id} + \nabla_x^\star\nabla_x\}^{-1}\Pi_v f$, which completes the proof. □

Establishing **A**3-(a) (referred to as microscopic coercivity in [21]) for the processes considered is fairly straightforward in the present framework.

[1] Note that the result is stated for functions $f \in \mathrm{C}^3_\mathrm{poly}(\mathbb{R}^d)$ but the proof can be easily extended to $f \in \mathrm{C}^2_\mathrm{poly}(\mathsf{X})$

Proposition 10. *Assume that $\mathcal{L}_i$, $i \in \{1,2\}$ given by (1) or (3), where $\mathcal{B}_k$ is defined in (4) satisfies **A** 1 with $\mathsf{C} = \mathrm{C}^2_{\mathrm{b}}(\mathsf{E})$. Assume in addition that **H** 1, **H** 2, **H** 3, **H** 4 **H** 5 and **H** 6 hold. Let $\mathcal{S}$ be the symmetric part of $\mathcal{L}_i$ defined by (16). Then **A** 3-(a) is satisfied with $\lambda_v = \underline{\lambda}$ and $\mathsf{C} = \mathrm{C}^2_{\mathrm{b}}(\mathsf{E})$.*

Proof. From **H**5-(c) and **H**6, it holds that for any $f \in \mathrm{C}^2_{\mathrm{b}}(\mathsf{E})$, we have

$$- \left\langle \lambda_{\mathrm{ref}} m_2^{1/2} \mathcal{R}_v f, f \right\rangle_2 \geq \underline{\lambda} m_2^{1/2} \left\langle (\mathrm{Id} - \Pi_v) f, f \right\rangle_2 \ . \tag{35}$$

In addition, any $f \in \mathrm{C}^2_{\mathrm{b}}(\mathsf{E})$ satisfies $\max_{k \in \{1,\ldots,K\}} \left\| v^\top F_k f \right\|_2 < +\infty$ by **H**1,(10) and (11), then by **H**3 for any $k \in \{1, \ldots, K\}$, $\sup_{k\in\{1,\ldots,K\}} \|\lambda_k^{\mathrm{e}} f\|_2 < +\infty$. Therefore, using the Cauchy-Schwarz inequality, that $\mathcal{B}_k$ is a symmetric involution on $\mathrm{L}^2(\mu)$ by **H**4, and $\mathcal{B}_k \lambda_k^{\mathrm{e}} = \lambda_k^{\mathrm{e}}$ by definition (28), we obtain for any $k \in \{1, \ldots, K\}$ and $f \in \mathrm{C}^2_{\mathrm{b}}(\mathsf{E})$,

$$\langle \lambda_k^{\mathrm{e}} \mathcal{B}_k f, f \rangle_2 \leq \|(\lambda_k^{\mathrm{e}})^{1/2} f\|_2 \|(\lambda_k^{\mathrm{e}})^{1/2} \mathcal{B}_k f\|_2 = \|(\lambda_k^{\mathrm{e}})^{1/2} f\|_2^2 \ .$$

As a result, we deduce $\langle \lambda_k^{\mathrm{e}} (\mathrm{Id} - \mathcal{B}_k) f, f \rangle_2 \geq 0$. Combining this result and (35) in the expression for $\mathcal{S}$ given in (30) in Proposition 8 completes the proof. □

The following lemma establishes equivalence between **A**3-(b) and the Poincaré inequality **H**1 , which allows one to refer to the expansive body of literature on the topic and implies dependence on the properties of the potential U only.

Proposition 11. *Assume that $\mathcal{L}_i$, $i \in \{1,2\}$ given by (1) or (3), where $\mathcal{B}_k$ as in (4) satisfies **A** 1 with $\mathsf{C} = \mathrm{C}^2_{\mathrm{b}}(\mathsf{E})$. Assume in addition that **H** 1, **H** 2, **H** 3, **H** 4 **H** 5 and **H** 6 hold. Let $\mathcal{T}_i$ be the anti-symmetric part of $\mathcal{L}_i$ defined by (16) and $\mathcal{A}_i$ be defined by (17) relative to $\mathcal{T}_i$. Then, **A** 3-(b), i.e. (19), holds with*

$$\lambda_x = C_{\mathrm{P}} / (1 + C_{\mathrm{P}}) \ . \tag{36}$$

Proof. From the assumed Poincaré inequality (8) we have for any $f \in \mathrm{C}^1_{\mathrm{b}}(\mathsf{E})$

$$\left\| m_2^{-1/2} \mathcal{D} \Pi_v f \right\|_2^2 = \|\nabla_x \Pi_v f\|_2^2 \geq C_{\mathrm{P}} \|\Pi_v f\|_2^2 \ .$$

Then, by definition of $\overline{\mathcal{D}\Pi_v}$ this inequality holds also for any $f \in \mathrm{D}(\overline{\mathcal{D}\Pi_v})$ replacing $\mathcal{D}\Pi_v f$ by $\overline{\mathcal{D}\Pi_v} f$. Therefore, we obtain since $(\mathcal{D}\Pi_v)^{\star\star} = \overline{\mathcal{D}\Pi_v}$ that for any $f \in \mathrm{D}((\mathcal{D}\Pi_v)^\star \overline{\mathcal{D}\Pi_v})$,

$$\left\langle f, m_2^{-1} (\mathcal{D}\Pi_v)^\star \overline{\mathcal{D}\Pi_v} f \right\rangle_2 \geq C_{\mathrm{P}} \|\Pi_v f\|_2^2 \ . \tag{37}$$

In addition by [49, Theorem 5.1.9], $(\mathcal{D}\Pi_v)^\star \overline{\mathcal{D}\Pi_v}$ is a self-adjoint operator. These results and (37) imply that $\mathrm{Spec}(m_2^{-1} (\mathcal{D}\Pi_v)^\star \overline{\mathcal{D}\Pi_v}) \subseteq [C_{\mathrm{P}}, \infty)$ by [16, Theorem 4.3.1].

On the other hand, since by Lemma 9-(a), $\overline{\mathcal{D}\Pi_v} = \overline{\mathcal{T}_i \Pi_v}$, we have $(\mathcal{D}\Pi_v)^\star = (\mathcal{T}_i \Pi_v)^\star$ and

$$\mathcal{A}_i = - \left(m_2 \, \mathrm{Id} + (\mathcal{D}\Pi_v)^\star \overline{\mathcal{D}\Pi_v} \right)^{-1} (\mathcal{D}\Pi_v)^\star \ .$$

Therefore, for any $f \in \mathrm{D}((\mathcal{D}\Pi_v)^\star \overline{\mathcal{D}\Pi_v})$,

$$- \overline{\mathcal{A}}_i \, \overline{\mathcal{D}\Pi_v} f = - \mathcal{A}_i \overline{\mathcal{D}\Pi_v} f = \left(m_2 \, \mathrm{Id} + (\mathcal{D}\Pi_v)^\star \overline{\mathcal{D}\Pi_v} \right)^{-1} (\mathcal{D}\Pi_v)^\star \overline{\mathcal{D}\Pi_v} f = \Phi\left(m_2^{-1} (\mathcal{D}\Pi_v)^\star \overline{\mathcal{D}\Pi_v} \right) f \ ,$$

where $\Phi(z) = z/(1+z)$. Since $\mathrm{D}((\mathcal{D}\Pi_v)^\star \overline{\mathcal{D}\Pi_v})$ is a core for $\overline{\mathcal{D}\Pi_v}$ by [49, Theorem 5.1.9.], from the spectral mapping theorem [16, Theorem 2.5.1, Corollary 2.5.4], and the fact that $\Phi \colon [0, \infty) \to [0, 1]$

is non-decreasing, we get that $-\overline{\mathcal{A}}_i\,\overline{\mathcal{D}\Pi_v}$ can be extended on $\mathrm{L}^2(\mu)$ as a self-adjoint bounded operator $\mathcal{E}$ and $\mathrm{Spec}(\mathcal{E}) \subseteq [\Phi(C_{\mathrm{P}}), 1)$.

Finally, from the fact that Π_v is a projector, we deduce from Lemma 3-(b) that $-\overline{\mathcal{A}}_i\mathcal{T}_i\Pi_v f = -\Pi_v\overline{\mathcal{A}}_i\,\overline{\mathcal{D}\Pi_v}\Pi_v f = \Pi_v\mathcal{E}\Pi_v f$ for any $f \in \mathrm{C}^2_{\mathrm{b}}(\mathsf{E}) \subset \mathrm{D}(\overline{\mathcal{D}\Pi_v})$ and therefore, we get that for any $f \in \mathrm{C}^2_{\mathrm{b}}(\mathsf{E})$

$$-\left\langle \Pi_v f, \overline{\mathcal{A}}\mathcal{T}_i\Pi_v f\right\rangle_2 = \langle \Pi_v f, \mathcal{E}\Pi_v f\rangle_2 \geq \frac{C_{\mathrm{P}}}{1+C_{\mathrm{P}}}\left\|\Pi_v f\right\|_2^2 = \lambda_x \left\|\Pi_v f\right\|_2^2 \ ,$$

which concludes the proof. □

A3-(c) is usually a more involved condition to check. For $f \in \mathrm{L}^2(\mu)$ denote by

$$u_f = m_2^{-1}(\mathrm{Id} + \nabla_x^\star\nabla_x)^{-1}\Pi_v f \ . \tag{38}$$

In the scenarios considered here, condition **A** 3-(c) relies on estimates of $\|u_f\|_2$, $\|\nabla_x u_f\|_2$ and $\left\|\nabla_x^2 u_f\right\|_2$ which are obtained by noticing that by definition u_f is solution of the following partial differential equation

$$m_2(\mathrm{Id} + \nabla_x^\star\nabla_x)u_f = \Pi_v f \ .$$

In the next section, we show how general, but potentially rough, estimates can be obtained, while in Section 5 we show how tighter bounds can be obtained in specific scenarios where we can take advantage of the structure at hand, in particular when interested in the scaling properties of the algorithm with d.

3.3 Computation of R_0 in the general setting

In all this section, we consider u_f defined for any $f \in \mathrm{L}^2(\mu)$ by (38). Recall that from Lemma 9-(d), if $f \in \mathrm{C}^2_{\mathrm{b}}(\mathsf{E})$ then $u_f \in \mathrm{C}^3_{\mathrm{poly}}(\mathbb{R}^d)$ and satisfies (33).

Lemma 12. *Assume that $\mathcal{L}_i$, $i \in \{1,2\}$ given by (1) or (3), where $\mathcal{B}_k$ is given in (4), satisfies **A** 1 with $\mathsf{C} = \mathrm{C}^2_{\mathrm{b}}(\mathsf{E})$. Assume in addition that **H**1, **H**2, **H**3, **H**4 **H**5 and **H**6 hold. Let $\mathcal{S}$ be the symmetric part of $\mathcal{L}_i$ defined by (16) and the operator $\mathcal{A}_i$ defined by (17) relative to $\mathcal{T}_i$.*

(a) For any $f \in \mathrm{C}^2_{\mathrm{b}}(\mathsf{E})$,

$$|\left\langle \overline{\mathcal{A}}_i\mathcal{S}(\mathrm{Id} - \Pi_v)f, f\right\rangle_2| \leq \|(\mathrm{Id} - \Pi_v)f\|_2\|(\mathrm{Id} - \Pi_v)\tilde{\mathcal{S}}\mathcal{A}_i^\star f\|_2 \ ,$$

where $\tilde{\mathcal{S}}$ is given by (30).

(b) For any $f \in \mathrm{C}^2_{\mathrm{b}}(\mathsf{E})$,

$$\|(\mathrm{Id} - \Pi_v)\tilde{\mathcal{S}}\mathcal{A}_i^\star f\|_2 = \|\mathbf{G}^\top\nabla_x u_f\|_2 \ , \tag{39}$$

with $\mathbf{G}$ given for any $(x,v) \in \mathsf{E}$ by

$$\mathbf{G}(x,v) = \sum_{k=1}^K \lambda_k^{\mathrm{e}}(x,v)\big(\mathrm{n}_k^\top(x)v\big)\mathrm{n}_k + m_2^{1/2}\lambda_{\mathrm{ref}}(x)v \ , \tag{40}$$

and u_f, $\{\lambda_k^{\mathrm{e}} : \mathsf{E} \to \mathbb{R}_+ \,:\, k \in \{1,\ldots,K\}\}$ are defined by (38) and (28) respectively. In addition

$$\|\mathbf{G}^\top \nabla_x u_f\|_2 \le m_2\big(\|\lambda_{\mathrm{ref}}\nabla_x u_f\|_2 + c_\varphi K \|\nabla_x u_f\|_2\big) + C_\varphi \sqrt{2m_{2,2} + 3(m_4 - m_{2,2})_+} \sum_{k=1}^K \|F_k^\top \nabla_x u_f\|_2 \; . \quad (41)$$

Proof. We only consider the case $i = 2$ since the case $i = 1$ is obtained by taking $F_0 = 0$.

(a) By Lemma 3-(b), $\overline{\mathcal{A}}_i$ is a bounded operator. Therefore, we have for any $f \in \mathrm{C}^2_{\mathrm{b}}(\mathsf{E})$ that $\langle \overline{\mathcal{A}}_i \mathcal{S}(\mathrm{Id} - \Pi_v) f, f\rangle_2 = \langle \mathcal{S}(\mathrm{Id} - \Pi_v) f, \mathcal{A}_i^\star f\rangle_2$. Then, by Lemma 9-(d), we have that $\mathcal{A}_i^\star f = -v^\top \nabla_x u_f$, with $u_f \in \mathrm{C}^3_{\mathrm{poly}}(\mathsf{E})$. This result, Proposition 8-(c), and the fact that $\mathrm{Id} - \Pi_v$ is an orthogonal projector imply that

$$\big\langle \overline{\mathcal{A}}_i \mathcal{S}(\mathrm{Id} - \Pi_v) f, f \big\rangle_2 = \big\langle (\mathrm{Id} - \Pi_v) f, (\mathrm{Id} - \Pi_v)\tilde{\mathcal{S}}\mathcal{A}_i^\star f \big\rangle_2 \; ,$$

with

$$\begin{aligned} \tilde{\mathcal{S}}\mathcal{A}_2^\star f &= -\left(\frac{1}{2}\sum_{k=1}^K \lambda_k^{\mathrm{e}}(\mathcal{B}_k - \mathrm{Id}) + m_2^{1/2}\lambda_{\mathrm{ref}}\mathcal{R}_v\right) v^\top \nabla_x u_f \\ &= \sum_{k=1}^K \lambda_k^{\mathrm{e}}\,(v^\top \mathrm{n}_k)(\mathrm{n}_k^\top \nabla_x u_f) + m_2^{1/2}\lambda_{\mathrm{ref}} v^\top \nabla_x u_f = \mathbf{G}^\top \nabla_x u_f \; , \end{aligned} \quad (42)$$

where we have used **H**5-(c) for the last equality. The proof is completed upon using the Cauchy-Schwarz inequality.

(b) Combining (42) and the fact that $\Pi_v \tilde{\mathcal{S}}\mathcal{A}_2^\star f = 0$ completes the proof of (39).

We now show (41) for any $f \in \mathrm{C}^2_{\mathrm{b}}(\mathsf{E})$. But it is a direct consequence of the triangle inequality, the definition of $\{\lambda_k^{\mathrm{e}} : \mathsf{E} \to \mathbb{R}_+ \,;\, k \in \{1, \ldots, K\}\}$ given in (28), **H**3, the Cauchy-Schwarz inequality, Lemma 38 and the identity $F_k = \mathrm{n}_k\,|F_k|$ for any $k \in \{1, \ldots, K\}$:

$$\begin{aligned} \|\mathcal{S}\mathcal{A}_2^\star f\|_2 &\le m_2^{1/2}\|\lambda_{\mathrm{ref}} v^\top \nabla_x u_f\|_2 + \sum_{k=1}^K \Big\{ C_\varphi \|(v^\top \mathrm{n}_k)^2\, F_k^\top \nabla_x u_f\|_2 + c_\varphi m_2^{1/2}\|(v^\top \mathrm{n}_k)\,\mathrm{n}_k^\top \nabla_x u_f\|_2 \Big\} \\ &= m_2\|\lambda_{\mathrm{ref}}\nabla_x u_f\|_2 + m_2 c_\varphi K \|\nabla_x u_f\|_2 + C_\varphi\sqrt{2m_{2,2} + 3(m_4 - m_{2,2})_+} \sum_{k=1}^K \|F_k^\top \nabla_x u_f\|_2. \end{aligned}$$

□

Lemma 13. *Assume that $\mathcal{L}_i$, $i \in \{1, 2\}$ given by (1) or (3), where $\mathcal{B}_k$ is given in (4), satisfies **A** 1 with $\mathsf{C} = \mathrm{C}^2_{\mathrm{b}}(\mathsf{E})$. Assume in addition that **H**1, **H**2, **H**3, **H**4 **H**5 and **H**6 hold. Let $\mathcal{T}_i$ be the anti-symmetric part of $\mathcal{L}_i$ defined by (16) and the operator $\mathcal{A}_i$ defined by (17) relative to $\mathcal{T}_i$. Then,*

(a) For any $f \in \mathrm{C}^2_{\mathrm{b}}(\mathsf{E})$, we get

$$|\big\langle \overline{\mathcal{A}}_i \mathcal{T}_i (\mathrm{Id} - \Pi_v) f, f \big\rangle_2| \le \|(\mathrm{Id} - \Pi_v) f\|_2 \|(\mathrm{Id} - \Pi_v)\tilde{\mathcal{T}}_i \mathcal{A}_i^\star f\|_2 \; ,$$

where $\tilde{\mathcal{T}}_i$ is given in (29).

(b) *For any* $f \in \mathrm{C}^2_{\mathrm{b}}(\mathsf{E})$

$$\|(\mathrm{Id} - \Pi_v)\tilde{\mathcal{T}}\mathcal{A}_i^\star f\|_2 = 2m_{2,2}\|\mathbf{M}\|_2^2 + 3(m_4 - m_{2,2})\|\mathrm{diag}(\mathbf{M})\|_2^2 \,, \tag{43}$$

with

$$\mathbf{M} = \nabla_x^2 u_f + \sum_{k=1}^K (F_k^\top \nabla_x u)\mathrm{n}_k\mathrm{n}_k^\top \,, \tag{44}$$

and u_f *defined by* (38).

Remark 14. *A general, but potentially rough, bound on the right hand side of* (43) *can be obtained as follows. From the fact that* $\|\mathrm{diag}(\mathbf{M})\|_2 \leq \|\mathbf{M}\|_2$, *it holds that*

$$\|(\mathrm{Id} - \Pi_v)\tilde{\mathcal{T}}_i\mathcal{A}_i^\star f\|_2 \leq \sqrt{2m_{2,2} + 3(m_4 - m_{2,2})_+}\|\mathbf{M}\|_2$$

where from the triangle inequality and the property $|\mathrm{n}_k(x)\mathrm{n}_k(x)^\top| = 1$

$$\|\mathbf{M}\|_2 \leq \|\nabla_x^2 u_f\|_2 + \sum_{k=1}^K \|F_k^\top \nabla_x u_f\|_2 \,.$$

Remark 15. *Specific scenarios lead to simplifications of these bounds and the bounds in Lemma 19:*

(a) *from Lemma 36 for radial distributions* $m_4 = m_{2,2}$ *leading to a simplification of this bound,*

(b) *further if* ν *is the centred normal distribution of covariance* $m_2\,\mathrm{I}_d$, *then* $m_{2,2} = m_2^2$, *leading to further simplifications,*

(c) *if* $K = 0$, *and hence* $F_0 = \nabla_x U$, *the scenario considered by [21], then one finds that the bound depends on* $\left\|\nabla_x^2 u_f\right\|_2$ *only.*

Proof. We proceed as in the proof of Lemma 12. We only consider the case $i = 2$ since the case $i = 1$ is obtained by taking $F_0 = 0$.

(a) By Lemma 3-(b), $\overline{\mathcal{A}}_2$ is a bounded operator. Therefore, we have for any $f \in \mathrm{C}^2_{\mathrm{b}}(\mathsf{E})$ that $\langle \overline{\mathcal{A}}_2\mathcal{T}_2(\mathrm{Id} - \Pi_v)f, f\rangle_2 = \langle \mathcal{T}_2(\mathrm{Id} - \Pi_v)f, \mathcal{A}_2^\star f\rangle_2$. Then, by Lemma 9-(d), we have that $\mathcal{A}_2^\star f = -v^\top \nabla_x u_f$, with $u_f \in \mathrm{C}^3_{\mathrm{poly}}(\mathsf{E})$. This result, Proposition 8-(c), the fact that $\mathrm{Id} - \Pi_v$ is an orthogonal projector and $F_k = \mathrm{n}_k|F_k|$, imply that for any

$$\left\langle \overline{\mathcal{A}}_2\mathcal{T}_2(\mathrm{Id} - \Pi_v)f, f\right\rangle_2 = \left\langle (\mathrm{Id} - \Pi_v)f, (\mathrm{Id} - \Pi_v)\tilde{\mathcal{T}}_2\mathcal{A}_2^\star f\right\rangle_2 \,,$$

with for any $(x, v) \in \mathsf{E}$,

$$\begin{aligned} -\tilde{\mathcal{T}}_2\mathcal{A}_2^\star f(x,v) &= v^\top \nabla_x^2 u_f(x) v - m_2 F_0^\top(x)\nabla_x u_f(x) - \sum_{k=1}^K (v^\top F_k(x))\left(\mathrm{n}_k(x)\mathrm{n}_k(x)^\top v\right)^\top \nabla_x u_f(x) \\ &= v^\top \mathbf{M}(x) v - m_2 F_0^\top(x)\nabla_x u_f(x) \,. \end{aligned} \tag{45}$$

The proof is completed upon using the Cauchy-Schwarz inequality.

(b) By (45), we obtain that for any $f \in \mathrm{C}_{\mathrm{b}}^2(\mathsf{E})$, $(x,v) \in \mathsf{E}$,

$$-(\mathrm{Id} - \Pi_v)\tilde{\mathcal{T}}_2\mathcal{A}_i^\star f(x,v) = v^\top \mathbf{M}(x)v - m_2 \operatorname{Tr}(\mathbf{M}(x)) .$$

Combining this result and Lemma 38, we deduce

$$\begin{aligned}\|(\mathrm{Id} - \Pi_v)\tilde{\mathcal{T}}_2\mathcal{A}_i^\star f\|_2^2 &= 2m_{2,2}\|\mathbf{M}\|_2^2 + 3(m_4 - m_{2,2})\|\mathrm{diag}(\mathbf{M})\|_2^2 \\ &\le \left[2m_{2,2} + 3(m_4 - m_{2,2})_+\right]\|\mathbf{M}\|_2^2 ,\end{aligned}$$

which completes the proof. □

Remark 16. *Combining Corollary 29 and Corollary 35 in Appendix C, by definition of u_f in (38) and using **H**6, we obtain that $m_2\|\nabla_x u_f\|_2 \le 2^{-1/2}\|\Pi_v f\|_2$,*

$$\begin{aligned}\sum_{k=1}^K \|F_k^\top \nabla_x u_f\|_2 &\le \frac{2^{1/2}\kappa_1}{m_2\kappa_2}\sum_{k=1}^K a_k\|\Pi_v f\|_2 , \\ m_2\|\lambda_{\mathrm{ref}}\nabla_x u_f\|_2 &\le \underline{\lambda}\left\{2^{-1/2} + \frac{2^{1/2}c_\lambda\kappa_1}{\kappa_2}\right\}\|\Pi_v f\|_2 .\end{aligned}$$

4 Postponed proofs

4.1 Proof of Theorem 1

In this section we prove that **A**2 and **A**3 holds for the dynamics described in Section 2 in order to obtain Theorem 1 as a consequence of the abstract Theorem 4. Under the assumptions of the theorem, we can set C to be $\mathrm{C}_{\mathrm{b}}^2(\mathsf{E})$. **A**2 and **A**3-(d) hold by Lemma 9-(a). **A**3-(a) follows from Proposition 10 with $\lambda_v = \underline{\lambda}$. **A**3-(b) follows from Proposition 11 with $\lambda_x = C_{\mathrm{P}}/(1 + C_{\mathrm{P}})$. **A**3-(e) follows from Proposition 8-(b). We are left with checking **A**3-(c). By Lemma 12-(b), Lemma 13-(b), Remark 14, we get setting $m = \sqrt{2m_{2,2} + 3(m_4 - m_{2,2})_+}$, for any $f \in \mathrm{C}_{\mathrm{b}}^2(\mathsf{E})$ that

$$\begin{aligned}&\left\|\tilde{\mathcal{S}}\mathcal{A}_i^\star f\right\|_2 + \left\|(\mathrm{Id} - \Pi_v)\tilde{\mathcal{T}}_i\mathcal{A}_i^\star f\right\|_2 \\ &\quad\le m\left\{\|\nabla_x^2 u_f\|_2 + (1 + C_\varphi)\sum_{k=1}^K \|F_k^\top\nabla_x u_f\|_2\right\} + m_2\|\lambda_{\mathrm{ref}}\nabla_x u_f\|_2 + m_2 c_\varphi K\|\nabla_x u_f\|_2 \\ &\quad\le \left[\frac{m}{m_2}\left\{\frac{2^{1/2}(1 + C_\varphi)\kappa_1}{\kappa_2}\sum_{k=1}^K a_k + \kappa_1\right\} + \frac{\underline{\lambda}}{2^{1/2}}\left\{1 + \frac{2c_\lambda\kappa_1}{\kappa_2}\right\} + \frac{c_\varphi K}{2^{1/2}}\right]\|\Pi_v f\|_2 ,\end{aligned}$$

where we have used that $\left\|\nabla_x^2 u_f\right\|_2 \le m_2^{-1}\kappa_1\left\|\Pi_v f\right\|_2$ by Proposition 33 in Appendix C and Remark 16, with κ_1 and κ_2 given in (69) and (72) respectively. The proof of **A**3-(c) is then completed using Lemma 13-(a) and Lemma 12-(a).

4.2 Proof of Lemma 6

Proof of Lemma 6. Fix $\lambda_x \in (0,1)$.

(a) Using that $t \mapsto (1+t)/\left[(1+t)^2 + R_0^2\right]$ is nondecreasing on $\mathbb{R}_+$, we obtain that for any $R_0 \ge 4 + 2\sqrt{3}$, (27) is satisfied.

(b) Since for any $a > 0$, $s \mapsto (s+a)/(s-a)$ for $s > a$ is nonincreasing, we deduce from above that for $R_0 \geq (4+2\sqrt{3}) \vee (\lambda_v/2^{1/2})$,

$$A(\epsilon_0)^2 \leq \frac{4R_0 + 2^{1/2}\lambda_v}{4R_0 - 2^{1/2}\lambda_v} \leq \frac{2^{3/2}\lambda_v + 2^{1/2}\lambda_v}{2^{3/2}\lambda_v - 2^{1/2}\lambda_v} < 3^{1/2} \; .$$

For the second part of the statement, first note that

$$\Lambda(\epsilon) = 2^{-1}[1-\epsilon(1-\lambda_x)]\left[1 - \left(1-\epsilon b_\Lambda(\epsilon)\right)^{1/2}\right] \; ,$$

where $b_\Lambda(\epsilon) = \left[4\lambda_x(1-\epsilon) - \epsilon R_0^2\right]/[1-\epsilon(1-\lambda_x)]^2 \in \left[0, \epsilon^{-1}\right]$ for $\epsilon \leq (2^{1/2}\lambda_v)^{-1} \wedge \{4\lambda_x/(4\lambda_x + R_0^2)\}$. Using that for any $a \in [0,1]$, $a/2 \leq 1-(1-a)^{1/2} \leq a$ we deduce that for $\epsilon \leq (2^{1/2}\lambda_v)^{-1} \wedge \{4\lambda_x/(4\lambda_x + R_0^2)\}$,

$$4^{-1}[1-\epsilon(1-\lambda_x)]\epsilon b_\Lambda(\epsilon) \leq \Lambda(\epsilon) \leq 2^{-1}[1-\epsilon(1-\lambda_x)]\epsilon b_\Lambda(\epsilon) \; .$$

Further for $R_0 \geq (4+2\sqrt{3}) \vee (\lambda_v/2^{1/2})$ we have $\epsilon_0 \leq (2^{1/2}\lambda_v)^{-1} \wedge \{3\lambda_x/(4\lambda_x + R_0^2)\}$ from Theorem 4-(b), leading to

$$\lambda_x/[1-\epsilon_0(1-\lambda_x)]^2 \leq b_\Lambda(\epsilon_0) \leq 4\lambda_x/[1-\epsilon_0(1-\lambda_x)]^2 \; ,$$

and consequently, using (27),

$$\epsilon_0\lambda_x/4 \leq \Lambda(\epsilon_0) \leq 2\lambda_x\epsilon_0/[1-2(1-\lambda_x)/(4+R_0^2)] \leq 4\lambda_x\epsilon_0 \; ,$$

where we have used that $\lambda_x \leq 1$ for the last inequality. Finally we note that from (27)

$$\frac{2}{3} \leq \frac{1}{1+2^{3/2}\lambda_v/(4+R_0^2)} \leq \frac{1}{1+2^{1/2}\lambda_v\epsilon_0} \leq 1 \; ,$$

where the leftmost inequality follows from the fact that for $2^{1/2}R_0 \geq \lambda_v$

$$\frac{2^{3/2}\lambda_v}{4+R_0^2} \leq \frac{2^{3/2}\lambda_v}{4+2^{-1}\lambda_v^2} \leq 1/2 \; .$$

□

4.3 Proof of Corollary 2

Proof of Theorem 2. Since $\lambda_v = \underline{\lambda}$ and $R_0 \geq (4+2\sqrt{3}) \vee (\underline{\lambda}/2^{1/2})$ by Theorem 1, from Theorem 4 and Lemma 6, $A < 3^{1/2}$ while with $\lambda_x = C_{\mathrm{P}}/(1+C_{\mathrm{P}})$

$$\underline{\lambda}\lambda_x m_2^{1/2}\epsilon_0/6 \leq \alpha(\epsilon_0) \quad \text{with} \quad \lambda_x/(1+R_0^2) \leq \epsilon_0 \leq 2/(4+R_0^2) \; . \tag{46}$$

By (13), if $c_1, c_2, \|a\|_\infty, m_b$ are fixed, there exist $C_1^R(C_{\mathrm{P}}, c_1, c_2, \|a\|_\infty, m_b) > 0$, independent of $d, \underline{\lambda}$, c_λ, C_φ and c_φ such that

$$\overline{R}_0 \leq C_1^R(C_{\mathrm{P}}, c_1, c_2, \|a\|_\infty, m_b)\overline{R}_1 \; ,$$

where $\overline{R}_1 = c_\varphi K + (1+C_\varphi)d^{(1+\varpi)/2}K + \underline{\lambda}(1+c_\lambda d^{(1+\varpi)/2})$. Combining this bound with (46) concludes the proof. □

5 The Zig-Zag sampler–optimization

In this section, we specify our results in the case of the Zig-Zag sampler for which better estimates can be obtained, leading to better scaling properties with respect to d. The Zig-Zag process corresponds to the instantiation of (1) for which $F_0 = 0$, $K = d$, $F_i(x) = \partial_{x_i} U(x)\mathbf{e}_i$, $\mathrm{n}_i(x) = \mathbf{e}_i$, $\lambda_{\mathrm{ref}}(x) = \underline{\lambda} > 0$[2], for $i \in \{1, \ldots, d\}$ and $x \in \mathsf{X}$, and $\mathcal{R}_v = \Pi_v - \mathrm{Id}$. The corresponding generator takes the simplified form, for $f \in \mathrm{C}^2_{\mathrm{b}}(\mathsf{E})$ and any $(x, v) \in \mathsf{E}$

$$\mathcal{L}f(x,v) = v^\top \nabla_x f(x) + \sum_{i=1}^{d} \varphi\big(v_i \partial_{x_i} U(x)\big)\left[f\big(x, (\mathrm{Id} - 2\mathbf{e}_i\mathbf{e}_i^\top)v\big) - f(x,v)\right] + \lambda_{\mathrm{ref}}(x) m_2^{1/2} \mathcal{R}_v f(x,v) \; , \tag{47}$$

where $\varphi : \mathbb{R} \to \mathbb{R}_+$ is a continuous function and satisfies (12) in **H**3.

In the next two subsections we first consider general velocity distributions and then show how our results can be specialized to the scenario where $\mathsf{V} = \{-m_2^{1/2}, +m_2^{1/2}\}^d$ for $m_2 > 0$ and ν is the uniform distribution on V.

5.1 General velocity distribution

Theorem 17. *Consider the Zig-Zag process with generator defined by (47) with $\lambda_{\mathrm{ref}} = \underline{\lambda}$, $\mathcal{R}_v = \Pi_v - \mathrm{Id}$ and $\varphi : \mathbb{R} \to \mathbb{R}_+$ is a continuous function satisfying (12) in **H**3. Assume **A**1 with $\mathsf{C} = \mathrm{C}^2_{\mathrm{b}}(\mathsf{E})$, **H**1, **H**2, **H**4, **H**5, **H**6 hold and that there exists $c_3 \geq 0$ such that for any $g \in \mathrm{L}^2(\pi)^d$*

$$\left\langle g, \left[\nabla_x^2 U - \mathrm{diag}(\nabla_x^2 U)\right] g\right\rangle_2 \geq -c_3 \left\|g\right\|_2^2 \; . \tag{48}$$

Then, Theorem 4 holds with λ_x as in (36), $\lambda_v = \underline{\lambda}$ and

$$R_0 = \frac{(6m_4)^{1/2}(2 + C_\varphi)}{m_2} \left((1 + c_1/2)^{1/2} + 1 + (c_3/2)^{1/2}\right) + \frac{\underline{\lambda} + c_\varphi}{2^{1/2}} \; . \tag{49}$$

Remark 18. *From **H**1 we have for any $g \in \mathrm{L}^2(\pi)^d$*

$$\left\langle g, \nabla_x^2 U g\right\rangle_2 \geq -c_1 \left\|g\right\|_2^2$$

and therefore (48) holds if there exist $\bar{c}_1 > 0$ such that for any $g \in \mathrm{L}^2(\pi)^d$,

$$\left\langle g, \mathrm{diag}(\nabla_x^2 U) g\right\rangle_2 \leq \bar{c}_1 \left\|g\right\|_2^2 \; ,$$

which is itself implied by $\bar{c}_1 \,\mathrm{Id} \succeq \mathrm{diag}(\nabla_x^2 U(x))$ for all $x \in \mathsf{X}$, since $\mathrm{diag}(\nabla_x^2 U(x))$ is symmetric. Note that this is the case when $|\mathrm{diag}(\nabla_x^2 U(x))| \leq \bar{c}_1$ or $|\nabla_x^2 U(x)| \leq \bar{c}_1$ for all $x \in \mathsf{X}$, for example.

Proof. The proof is very similar to the proof Theorem 1 and follows from applying Theorem 4. Checking **A**2 and **A**3-(a)-(b)-(d)-(e) is identical to the work done in the proof of Theorem 1 with the constants $\lambda_v = \underline{\lambda}$ and λ_x given by (36). We are left with checking **A**3-(c). By the improved bounds from Lemma 19 and Lemma 20, we have for any $f \in \mathrm{C}^2_{\mathrm{b}}(\mathsf{E})$,

$$\begin{aligned} &\left\|\tilde{\mathcal{S}}\mathcal{A}^\star f\right\|_2 + \left\|(\mathrm{Id} - \Pi_v)\tilde{\mathcal{T}}\mathcal{A}^\star f\right\|_2 \\ &\qquad \leq (6m_4)^{1/2}(2 + C_\varphi)\left(\left\|\nabla_x^2 u_f\right\|_2 + \left\|\nabla_x^* \nabla_x u_f\right\|_2 + c_3^{1/2} \left\|\nabla_x u_f\right\|_2\right) + \left(\underline{\lambda} + c_\varphi\right) m_2 \left\|\nabla_x u_f\right\|_2 \; . \end{aligned}$$

[2] which corresponds to $c_\lambda = 0$ in **H**6

Using Proposition 33 and Corollary 35, we obtain that for any $f \in \mathrm{C}^2_{\mathrm{b}}(\mathsf{E})$,

$$\left\|(\mathrm{Id} - \Pi_v)\tilde{\mathcal{S}}\mathcal{A}^\star f\right\|_2 + \left\|(\mathrm{Id} - \Pi_v)\tilde{\mathcal{T}}\mathcal{A}^\star f\right\|_2 \\ \leq \left\{ \frac{(6m_4)^{1/2}(2 + C_\varphi)}{m_2}\left((1+c_1/2)^{1/2} + 1 + (c_3/2)^{1/2}\right) + \frac{\underline{\lambda} + c_\varphi}{2^{1/2}} \right\} \|\Pi_v f\|_2 \ ,$$

The proof is then completed by Lemma 12-(a) and Lemma 13-(a). □

We discuss in the following the dependence on the dimension of the convergence rate $\alpha(\epsilon_0)$ and the constant $A(\epsilon_0)$ given by Theorem 4 based on the constant provided by Theorem 17. Similarly to the general case, we need to impose some conditions on m_2, m_4. Here, we assume that $m_4^{1/2}/m_2$ does not depend on d, which holds in the case where ν is the uniform distribution on $\mathsf{V} = \{-1, 1\}^d$ or the d-dimensional zero-mean Gaussian distribution with covariance matrix I_d.

In the case where π is the i.i.d. product of one-dimensional distributions π_i on $(\mathbb{R}, \mathcal{B}(\mathbb{R}))$ associated with potentials $U_i : \mathbb{R} \to \mathbb{R}$ satisfying **H** 1, *i.e.* for any $x \in \mathsf{X}$, $U(x) = \sum_{i=1}^d U_i(x_i)$, $\nabla_x^2 U(x) = \mathrm{diag}(\nabla_x^2 U(x))$ for any $x \in \mathsf{X}$ and therefore (48) holds with $c_3 = 0$. Then, the convergence rate $\alpha(\varepsilon_0)$ and the constant $A(\varepsilon_0)$ in Theorem 4 do not depend on the dimension but only on the constants c_1, c_2, $\underline{\lambda}$, c_λ and C_{P} associated to each U_i.

Consider now the case where the potential U is strongly convex and gradient Lipschitz, *i.e.* there exist $m, L > 0$ such that $m\,\mathrm{I}_d \preceq \nabla_x^2 U(x) \preceq L\,\mathrm{I}_d$ for any $x \in \mathsf{X}$. Then, since for any $i \in \{1, \ldots, d\}$ and $x \in \mathsf{X}$, $\partial_{x_i,x_i} U(x) = \mathbf{e}_i^\top \nabla_x^2 U(x)\mathbf{e}_i \leq L$ by assumption, Remark 18 implies that (48) holds for $c_3 = L - m$. In addition, **H**1 holds with $c_1 = 0$ and $c_2 = L$ and by [4, Proposition 5.1.3, Corollary 5.7.2], U satisfies (8) with $C_{\mathrm{P}} = m$. Then, the convergence rate $\alpha(\varepsilon_0)$ and the constant $A(\varepsilon_0)$ in Theorem 4 do not depend on the dimension but only on L, m, $\underline{\lambda}$ and $\overline{\lambda}$. In addition, we observe that the larger $L - m$ is, the larger R_0 given in (49) is, which in turn make the convergence rate $\alpha(\varepsilon_0)$ worse since it is of order $\mathcal{O}(1/R_0^2)$ as $R_0 \to +\infty$ by Lemma 6. This result is expected in the Gaussian case $U(x) = x^\top \Sigma x$ for any $x \in \mathsf{X}$, since $L - m$ is the diameter of the set of eigenvalues of Σ which is a characterization of the conditioning of the problem.

Lemma 19. *Consider the Zig-Zag process with generator $\mathcal{L}$ defined by (47) with $\lambda_{\mathrm{ref}} = \underline{\lambda}$, $\mathcal{R}_v = \Pi_v - \mathrm{Id}$ and $\varphi : \mathbb{R} \to \mathbb{R}_+$ is a continuous function satisfying (12) in **H**3. Assume **A**1 with $\mathsf{C} = \mathrm{C}^2_{\mathrm{b}}(\mathsf{E})$, **H**1, **H**2, **H**4, **H**5, **H**6 and (48) hold. Let $\mathcal{S}$ and $\mathcal{T}$ be the symmetric and anti-symmetric parts of $\mathcal{L}$ respectively and $\mathcal{A}$ the operator defined by (17) relative to $\mathcal{T}$. Then for any $f \in \mathrm{C}^2_{\mathrm{b}}(\mathsf{E})$,*

$$\|(\mathrm{Id} - \Pi_v)\tilde{\mathcal{S}}\mathcal{A}^\star f\|_2 \\ \leq (6m_4)^{1/2} C_\varphi \left(\left\|\nabla_x^2 u_f\right\|_2 + \|\nabla_x^\star \nabla_x u_f\|_2 + c_3^{1/2}\|\nabla_x u_f\|_2 \right) + (\underline{\lambda} + c_\varphi) m_2 \|\nabla_x u_f\|_2 \ ,$$

where u_f is given by (38).

Proof. We use Lemma 12 and its notation, where $K = d$, for $k \in \{1, \ldots, d\}$, $F_k = \partial_{x_k} U$ and $\mathrm{n}_k = \mathrm{sgn}(\partial_{x_k} U)\mathbf{e}_k$. In this setting and by (40), it follows that for any $(x, v) \in \mathsf{E}$,

$$\mathbf{G}(x, v) = \sum_{k=1}^d \lambda_k^{\mathrm{e}}(x, v) v_k \mathbf{e}_k + \underline{\lambda} m_2^{1/2} v \ .$$

By the triangle inequality and since for $i,j\in\{1,\ldots,d\}$, $i\neq j$, $\int_{\mathsf{V}} g(v_i)g(v_j)v_iv_j\mathrm{d}\nu(v)=0$ by **H** 4-(c) for any even measurable bounded function $g:\mathbb{R}\to\mathbb{R}$, we get

$$\begin{aligned}\left\|\mathbf{G}^\top\nabla_x u_f\right\|_2 &\leq \left\|\textstyle\sum_{k=1}^d\{\varphi(v_k\partial_{x_k}U)+\varphi(-v_k\partial_{x_k}U)\}v_k\partial_{x_k}u_f\right\|_2+\underline{\lambda}m_2\left\|\nabla_x u_f\right\|_2\\ &=\left[\sum_{k=1}^d\left\|\{\varphi(v_k\partial_{x_k}U)+\varphi(-v_k\partial_{x_k}U)\}v_k\partial_{x_k}u_f\right\|_2^2\right]^{1/2}+\underline{\lambda}m_2\left\|\nabla_x u_f\right\|_2\ .\end{aligned}$$

Then by **H**3, **H**4-(c), the triangle inequality (on $\mathrm{L}^2(\mu)^d$) and since for any $i\in\{1,\ldots,d\}$, $\int_{\mathsf{V}} v_i^4\mathrm{d}\nu(v)=3m_4$ by **H**4-(d) we obtain

$$\begin{aligned}\left\|\mathbf{G}^\top\nabla_x u_f\right\|_2 &\leq \left[\sum_{k=1}^d\left\|(c_\varphi m_2^{1/2}+C_\varphi\left|v_k\partial_{x_k}U\right|)v_k\partial_{x_k}u_f\right\|_2^2\right]^{1/2}+\underline{\lambda}m_2\left\|\nabla_x u_f\right\|_2\\ &\leq c_\varphi m_2^{1/2}\left[\sum_{k=1}^d\left\|v_k\partial_{x_k}u_f\right\|_2^2\right]^{1/2}+C_\varphi\left[\sum_{k=1}^d\left\|\left|v_k\partial_{x_k}U\right|v_k\partial_{x_k}u_f\right\|_2^2\right]^{1/2}+\underline{\lambda}m_2\left\|\nabla_x u_f\right\|_2\\ &\leq (c_\varphi+\underline{\lambda})m_2\left\|\nabla_x u_f\right\|_2+C_\varphi(3m_4)^{1/2}\left[\sum_{k=1}^d\left\|\partial_{x_k}U\partial_{x_k}u_f\right\|_2^2\right]^{1/2}\ . \end{aligned}\tag{50}$$

To bound the sum we note that for $k\in\{1,\ldots,d\}$ $\partial_{x_k}U\partial_{x_k}u_f=\partial_{x_k}^2u_f+\partial_{x_k}^*\partial_{x_k}u_f$ by Lemma 31-(a), which together with the fact $(a+b)^2\leq 2(a^2+b^2)$ leads to

$$\left\|\partial_{x_i}U\partial_{x_i}u_f\right\|_2^2\leq 2\left(\left\|\partial_{x_i}^2u_f\right\|_2^2+\left\|\partial_{x_i}^*\partial_{x_i}u_f\right\|_2^2\right)\ .$$

Then, using that for $a,b\geq 0$ $\sqrt{a+b}\leq\sqrt{a}+\sqrt{b}$ twice and (54), we deduce

$$\begin{aligned}\left(\sum_{k=1}^d\left\|\partial_{x_k}U\partial_{x_k}u_f\right\|_2^2\right)^{1/2} &\leq 2^{1/2}\left\{\sum_{k=1}^d\left(\left\|\partial_{x_k}^2u_f\right\|_2^2+\left\|\partial_{x_k}^*\partial_{x_k}u_f\right\|_2^2\right)\right\}^{1/2}\\ &\leq 2^{1/2}\left\{\left(\sum_{k=1}^d\left\|\partial_{x_k}^2u_f\right\|_2^2\right)^{1/2}+\left(\sum_{k=1}^d\left\|\partial_{x_k}^*\partial_{x_k}u_f\right\|_2^2\right)^{1/2}\right\}\\ &\leq 2^{1/2}\left(\left\|\nabla_x^2u_f\right\|_2+\left\|\nabla_x^*\nabla_x u_f\right\|_2+c_3^{1/2}\left\|\nabla_x u_f\right\|_2\right)\ .\end{aligned}\tag{51}$$

Then combining (50) and (51) completes the proof by Lemma 12-(b). ☐

Lemma 20. *Consider the Zig-Zag process with generator $\mathcal{L}$ defined by (47) with $\lambda_{\mathrm{ref}}=\underline{\lambda}$, $\mathcal{R}_v=\Pi_v-\mathrm{Id}$ and $\varphi:\mathbb{R}\to\mathbb{R}_+$ a continuous function satisfying (12) in **H**3. Assume **A**1 with $\mathsf{C}=\mathrm{C}_\mathrm{b}^2(\mathsf{E})$, **H**1, **H**2, **H**4, **H**5, **H**6 and (48) hold. Let $\mathcal{T}$ be the anti-symmetric part of $\mathcal{L}$ and $\mathcal{A}$ the operator defined by (17) relative to $\mathcal{T}$. Then for any $f\in\mathrm{C}_\mathrm{b}^2(\mathsf{E})$*

$$\left\|(\mathrm{Id}-\Pi_v)\tilde{\mathcal{T}}\mathcal{A}^\star f\right\|_2\leq[6(4m_4-m_{2,2})]^{1/2}\left(\left\|\nabla_x^2u_f\right\|_2+\left\|\nabla_x^*\nabla_x u_f\right\|_2+c_3^{1/2}\left\|\nabla_x u_f\right\|_2\right)\ ,$$

where u_f is defined by (38).

Proof. We use Lemma 13 and its notations, where $K = d$, for $k \in \{1,\dots,d\}$, $F_k = \partial_{x_k} U \mathbf{e}_k$ and $\mathrm{n}_k = \mathrm{sgn}(\partial_{x_k} U)\mathbf{e}_k$. In this setting and by (44), it follows that

$$\mathbf{M}(x) = \nabla_x^2 u_f(x) + \mathrm{diag}\big(\nabla_x u_f \odot \nabla_x U\big),$$

Since $\|\mathbf{M}\|_2^2 = \|\mathrm{diag}(\mathbf{M})\|_2^2 + \|\mathbf{M} - \mathrm{diag}(\mathbf{M})\|_2^2$, we obtain

$$\begin{aligned} 2m_{2,2}\|\mathbf{M}\|_2^2 + 3(m_4 - m_{2,2})\|\mathrm{diag}(\mathbf{M})\|_2^2 &= 2m_{2,2}\|\mathbf{M} - \mathrm{diag}(\mathbf{M})\|_2^2 + (3m_4 - m_{2,2})\|\mathrm{diag}(\mathbf{M})\|_2^2 \\ &\le 2m_{2,2}\left\|\nabla_x^2 u_f\right\|_2^2 + (3m_4 - m_{2,2})\|\mathrm{diag}(\mathbf{M})\|_2^2 \ . \qquad (52) \end{aligned}$$

We now bound $\|\mathrm{diag}(\mathbf{M})\|_2^2$. First, we apply the triangle inequality and use Lemma 31-(a), to deduce that

$$\begin{aligned} &\|\mathrm{diag}(\mathbf{M})\|_{\mathrm{L}^2(\pi)}^2 = \sum_{k=1}^d \left\|2\partial_{x_k}^2 u_f - \partial_{x_k}^2 u_f + \partial_{x_k} U \partial_{x_k} u_f\right\|_2^2 \\ &\le \sum_{k=1}^d \left(2\left\|\partial_{x_k}^2 u_f\right\|_2 + \left\|-\partial_{x_k}^2 u_f + \partial_{x_k} U \partial_{x_k} u_f\right\|_2\right)^2 \le \sum_{k=1}^d \left(8\left\|\partial_{x_k}^2 u_f\right\|_2^2 + 2\left\|\partial_{x_k}^* \partial_{x_k} u_f\right\|_2^2\right) \ , \qquad (53) \end{aligned}$$

where we have used for the last inequality that $(a+b)^2 \le 2a^2 + 2b^2$ for any $a, b \in \mathbb{R}$. By Lemma 31-(a), (68), (10) and the fact that $U \in \mathrm{C}^3_{\mathrm{poly}}(\mathsf{X})$ using **H**1, using that same reasoning as to establish (70), it holds for any $k \in \{1,\dots,d\}$,

$$\begin{aligned} \left\|\partial_{x_k}^\star \partial_{x_k} u_f\right\|_2^2 &= \left\|\partial_{x_k}^2 u_f\right\|_2^2 + \langle \partial_{x_k} u_f, \partial_{x_k, x_k} U\, \partial_{x_k} u_f\rangle_2 \ , \\ \|\nabla_x^* \nabla_x u_f\|_2^2 &= \left\|\nabla_x^2 u_f\right\|_2^2 + \left\langle \nabla_x u_f, \nabla_x^2 U \nabla_x u_f\right\rangle_2 \ . \end{aligned}$$

These identities and the condition (48) imply

$$\begin{aligned} &\sum_{i=1}^d \left\|\partial_{x_i}^* \partial_{x_i} u_f\right\|_2^2 = \left\|\mathrm{diag}\big(\nabla_x^2 u_f\big)\right\|_2^2 + \left\langle \nabla_x u_f, \mathrm{diag}\big(\nabla_x^2 U\big)\nabla_x u_f\right\rangle_2 \\ &\le \left\|\nabla_x^2 u_f\right\|_2^2 + \left\langle \nabla_x u_f, \mathrm{diag}\big(\nabla_x^2 U\big)\nabla_x u_f\right\rangle_2 \le \|\nabla_x^* \nabla_x u_f\|_2^2 - \left\langle \nabla_x u_f, \big(\nabla_x^2 U - \mathrm{diag}(\nabla_x^2 U)\big)\nabla_x u_f\right\rangle_2 \\ &\le \|\nabla_x^* \nabla_x u_f\|_2^2 + c_3\|\nabla_x u_f\|_2^2 \ . \qquad (54) \end{aligned}$$

Combining (53) and (54), we obtain

$$\|\mathrm{diag}(\mathbf{M})\|_2^2 \le 8\sum_{k=1}^d \left\|\partial_{x_k}^2 u_f\right\|_2^2 + 2(\|\nabla_x^* \nabla_x u_f\|_2^2 + c_3\|\nabla_x u_f\|_2^2) \ .$$

From this inequality, (52) and Lemma 13-(b), we deduce

$$\begin{aligned} \left\|(\mathrm{Id} - \Pi_v)\tilde{\mathcal{T}}\mathcal{A}^\star f\right\|_2^2 &\le 6(4m_4 - m_{2,2})\left\|\nabla_x^2 u_f\right\|_2^2 + 2(3m_4 - m_{2,2})\left(\|\nabla_x^* \nabla_x u_f\|_2^2 + c_3\|\nabla_x u_f\|_2^2\right) \\ &\le 6(4m_4 - m_{2,2})\left(\left\|\nabla_x^2 u_f\right\|_2 + \|\nabla_x^* \nabla_x u_f\|_2 + c_3^{1/2}\|\nabla_x u_f\|_2\right)^2 \ , \end{aligned}$$

since for $a, b, c \ge 0$, $a^2 + b^2 + c^2 \le (a+b+c)^2$. ∎

5.2 d-dimensional Radmacher distribution

We now consider the case $\mathsf{V} = \{-m_2^{1/2}, +m_2^{1/2}\}^d$ and ν is the uniform distribution on V which corresponds to the original setting of the Zig-Zag process. This process has been proved to be ergodic [8] even in the absence of refreshment, that is $\lambda_{\mathrm{ref}} = 0$. We note that in this scenario $m_4 = m_2^2/3$ and $m_{2,2} = m_2^2$ which leads to simplified expressions for the bounds in Lemma 19 and Lemma 20 upon revisiting their proofs. However this has no qualitative impact. In this section we show that hypocoercivity holds with our techniques for $\lambda_{\mathrm{ref}}(x) = 0$ for "most of X" for a particular type of partial refreshment update.

Consider the scenario where $\mathcal{R}_v$ is a mixture of the bounces $\{\mathcal{B}_k, k = 1, \ldots, d\}$, for any $f \in \mathrm{L}^2(\mu)$, $(x, v) \in \mathsf{E}$,

$$\lambda_{\mathrm{ref}} \mathcal{R}_v f(x,v) = \sum_{k=1}^{d} \lambda_{\mathrm{ref},k}(x) \left[f\left(x, v - 2v_k \mathbf{e}_k\right) - f(x,v) \right] , \tag{55}$$

with $\lambda_{\mathrm{ref},k} \colon \mathsf{X} \to \mathbb{R}_+$ for $k \in \{1, \ldots, d\}$ satisfying **H6**, and $\lambda_{\mathrm{ref}} = \sum_{k=1}^{d} \lambda_{\mathrm{ref},k}$, that is when the process refreshes, $k \in \{1, \ldots, d\}$ is chosen at random with probability proportional to $(\lambda_{\mathrm{ref},1}, \ldots, \lambda_{\mathrm{ref},d})$ and the component v_k of v is updated to $-v_k$.

Proposition 21. *Consider the Zig-Zag process with generator $\mathcal{L}$ and refreshment operator as in (47) and (55) respectively, with $\varphi : \mathbb{R} \to \mathbb{R}_+$ is a continuous function satisfying (12) in **H3**. Assume **A1** with $\mathsf{C} = \mathrm{C}_{\mathrm{b}}^2(\mathsf{E})$, **H1**, **H2**, **H4**, **H5**, **H6** and (48) hold. Let $\mathcal{S}$ be the symmetric part of $\mathcal{L}$ defined by (16).*

(a) the symmetric part of the generator is given for any $f \in \mathrm{C}_{\mathrm{b}}^2(\mathsf{E})$, $(x, v) \in \mathsf{E}$ by

$$\mathcal{S}f(x,v) = \sum_{k=1}^{d} \left\{ \frac{\varphi\big(v_k \partial_{x_k} U(x)\big) + \varphi\big(-v_k \partial_{x_k} U(x)\big)}{2} + m_2^{1/2} \lambda_{\mathrm{ref},k}(x) \right\} \left[f\left(x, v - 2v_k \mathbf{e}_k\right) - f(x,v) \right] ;$$

*(b) the microscopic coercivity condition **A3**-(a) is satisfied, i.e. for any $f \in \mathrm{C}_{\mathrm{b}}^2(\mathsf{E})$, $(x, v) \in \mathsf{E}$*

$$-\left\langle \mathcal{S}f, f \right\rangle_2 \geq \lambda_v m_2^{1/2} \left\| (\mathrm{Id} - \Pi_v) f \right\|_2^2 \quad \text{with} \quad \lambda_v = \min_{k \in \{1,\ldots,d\}, x \in \mathsf{X}} \left\{ \frac{|\partial_{x_k} U(x)|}{2} + \lambda_{\mathrm{ref},k}(x) \right\} . \tag{56}$$

Remark 22. *In other words **A3**-(a) holds if for any $\varepsilon > 0$, for all $k \in \{1, \ldots, d\}$, $\lambda_{\mathrm{ref},k}$ vanishes everywhere, except on $\{x \in \mathsf{X} : \exists k \in \{1, \ldots, d\} \mid |\partial_{x_k} U|(x) < \varepsilon\}$. We also note that a similar result holds for the case where $\mathcal{R}_v = \Pi_v - \mathrm{Id}$, that is **A3**-(a) holds whenever λ_{ref} vanishes everywhere, except on $\{x \in \mathsf{X} : \exists k \in \{1, \ldots, d\}, \mid |\partial_{x_k} U|(x) < \varepsilon\}$ for $\varepsilon > 0$.*

Proof. The first statement is a direct application of Proposition 8-(a). For the second statement, using that ν is the uniform distribution on $\mathsf{V} = \{-m_2^{1/2}, m_2^{1/2}\}^d$, from the polarization identity and since φ satisfies **H3**, we get for any $f \in \mathrm{C}_{\mathrm{b}}^2(\mathsf{E})$, setting $\varphi^{\mathrm{e}}(s) := \varphi(s) + \varphi(-s)$,

$$\begin{aligned} -\left\langle \mathcal{S}f, f \right\rangle_2 &= \frac{1}{2} \int_{\mathsf{E}} \sum_{k=1}^{d} \left\{ \frac{\varphi^{\mathrm{e}}(v_k \partial_{x_k} U(x))}{2} + m_2^{1/2} \lambda_{\mathrm{ref},k}(x) \right\} \left[f(x,v) - f\big(x, (\mathrm{Id} - 2\mathbf{e}_k \mathbf{e}_k^\top) v\big) \right]^2 \mathrm{d}\mu(x,v) \\ &\geq (\lambda_v m_2^{1/2}/2) \int_{\mathsf{E}} \sum_{k=1}^{d} \left[f(x,v) - f\big(x, (\mathrm{Id} - 2\mathbf{e}_k \mathbf{e}_k^\top) v\big) \right]^2 \mathrm{d}\mu(x,v) , \end{aligned} \tag{57}$$

where λ_v is defined in (56). Now by the Poincaré inequality for any $g \in \mathrm{L}^2_0(\nu)$, see e.g. [47, p. 52], it holds that

$$(1/2) \int_{\mathsf{V}} \sum_{k=1}^{d} \left[g(v) - g\big((\mathrm{Id} - 2\mathbf{e}_i \mathbf{e}_i^\top)v\big)\right]^2 \mathrm{d}\nu(v) \geq \int_{\mathsf{V}} \sum_{k=1}^{d} g^2(v)\, \mathrm{d}\nu(v) \; . \tag{58}$$

Now since for any $f \in \mathrm{C}^2_{\mathrm{b}}(\mathsf{E})$, $\langle \mathcal{S} f, f \rangle_2 = \langle \mathcal{S}(\mathrm{Id} - \Pi_v) f, (\mathrm{Id} - \Pi_v) f \rangle_2$ and for any $x \in \mathsf{X}$, $v \mapsto (\mathrm{Id} - \Pi_v) f(x, v) \in \mathrm{L}^2_0(\nu)$, then combining (57) and (58) and using Fubini's theorem concludes the proof of (56). □

6 Discussion and link to earlier work

As pointed out earlier the scenario $K = 0$ where $F_0 = \nabla_x U$ is considered in [21] where the authors establish hypercoercivity but also in [11, Theorem 3.9] where the authors establish geometric convergence, that is the existence of constants $A, \alpha > 0$ and a measurable function $V \colon \mathsf{E} \to \mathbb{R}_+$ satisfying $\mu\big(\{V = \infty\}\big) = 0$, such that for any $(x, v) \in \mathsf{E}$ and $t \geq 0$,

$$\| P_t\big((x, v), \cdot\big) - \mu(\cdot) \|_{\mathrm{TV}} \leq A V(x, v) \mathrm{e}^{-\alpha t} \; . \tag{59}$$

Similar results have been obtained in [18] and [24] for the Bouncy particle sampler and in [8] for the Zig-Zag process. All these methods rely on guessing such a suitable Lyapounov function V and establishing a so-called drift condition for this function, in conjunction with a minorization condition [42]. Here we have established $\mathrm{L}^2(\mu)$-exponential convergence, or equivalently that there exists an absolute $\mathrm{L}^2(\mu)$-absolute spectral gap [22, Proposition 22.3.2] (by considering the skeleton of the process) and is therefore μ-a.e. uniformly convergent by [22, Proposition 22.3.3 and Proposition 22.3.5], that is (59) holds with $V = \mathbf{1}$ and μ-a.e..

An advantage of our approach is that it provides explicit and relatively simple bounds in terms of interpretable quantities which, we show, are informative, and is in contrast with those on minorization and drift conditions in most scenarios. One exception is the study of BPS on the torus carried out in [24] for $U = 0$, using an appropriate coupling argument, which leads to a rate of convergence for the total variation distance with a favourable $\Theta(d^{1/2})$ scaling. Although we have shown that for the Zig-Zag sampler with Rademacher distribution λ_{ref} is not required to be bounded away from zero on X, the results of [8] hold with $\lambda_{\mathrm{ref}} = 0$. It would be interesting to further investigate whether our results can be specialized to consider the scenario $\lambda_{\mathrm{ref}} = 0$.

Although we have shown that the theory developed in this paper covers numerous scenarios in a unified set-up, various possible extensions are possible. For example we have restricted this first investigation to deterministic bounces of the type given in (4), but there does not seem to be any obstacle to the extension of our results to the more general set-ups such as considered in [55, 58, 44]. In the same vein, great parts of our calculations could be used to consider distributions of the velocity ν that are neither Gaussian, nor the uniform distribution on the hypersphere. For ν of density proportional to $\exp(-\mathrm{K}(v))$ with $\mathrm{K} : \mathbb{R}^d \to \mathbb{R}$ the Liouville operator involved in the definition of (3) would take the form $\nabla_v \mathrm{K}(v)^\top \nabla_x f(x, v) - m_2 F_0^\top \nabla_v f(x, v)$, leading to a different expression for $\mathcal{T}$. Such modified kinetic energies have been proposed to speed up the computation, introducing the Modified Langevin Dynamics for which convergence to equilibrium has been studied in [52].

A Optimization and estimates of the rate of convergence $\alpha(\epsilon)$

Consider the functions $R, \tilde{\alpha} : \mathbb{R}_+^* \to \mathbb{R}_+^*$ given for any $\epsilon \geq 0$ by

$$R(\epsilon) = [1 - \epsilon(1-\lambda_x)]^2 - 4\epsilon\lambda_x(1-\epsilon) + \epsilon^2 R_0^2 = R_1^2 \left(\epsilon - \frac{1+\lambda_x}{R_1^2}\right)^2 + 1 - \frac{(1+\lambda_x)^2}{R_1^2} > 0 \;, \quad (60)$$

$$\tilde{\alpha}(\epsilon) = \frac{\Lambda(\epsilon)}{1 + 2^{1/2}\lambda_v \epsilon} = \frac{1 - \epsilon(1-\lambda_x) - R^{1/2}(\epsilon)}{2(1 + 2^{1/2}\lambda_v\epsilon)} \;, \quad (61)$$

where

$$R_1^2 = (1+\lambda_x)^2 + R_0^2 \;, \quad (62)$$

and Λ is given in (21). We show that optimizing $\epsilon \mapsto \Lambda(\epsilon)$ is a good enough proxy for optimizing $\epsilon \mapsto \tilde{\alpha}(\epsilon)$, whose maximum is unique, but intractable. Since $\epsilon \mapsto \alpha(\epsilon)$ defined by (20) is proportional to $\epsilon \mapsto \tilde{\alpha}(\epsilon)$, the same conclusion holds for this function.

Lemma 23. *Let $\Lambda\colon \mathbb{R}_+ \to \mathbb{R}$ be defined by (21). Then with $\lambda_x \in (0,1)$ and $R_0 > 0$,*

(a) $\Lambda(\epsilon) \geq 0$ *for* $\epsilon \in \left[0, 4\lambda_x/(4\lambda_x + R_0^2)\right]$ *and* $\Lambda(0) = 0$.

(b) Λ *has first order derivative*

$$\Lambda'(\epsilon) = -(1/2)\left[(1-\lambda_x)R^{1/2}(\epsilon) + \epsilon R_1^2 - (1+\lambda_x)\right]R^{-1/2}(\epsilon) \;,$$

and $\Lambda'(0) = \lambda_x > 0$.

(c) $\Lambda\colon \mathbb{R}_+ \to \mathbb{R}$ *has a unique stationary point* ($\Lambda'(\epsilon_0) = 0$)

$$\epsilon_0 = \frac{(1+\lambda_x) - (1-\lambda_x)\left[R_0^2/(R_0^2 + 4\lambda_x)\right]^{1/2}}{(1+\lambda_x)^2 + R_0^2} > 0 \;, \quad (63)$$

such that $\Lambda(\epsilon_0) > 0$.

Proof. From (21) we see that $\Lambda(\epsilon) \geq 0$ requires

$$0 \leq \epsilon \leq \frac{1}{1-\lambda_x} \wedge \frac{4\lambda_x}{4\lambda_x + R_0^2} = \frac{4\lambda_x}{4\lambda_x + R_0^2} \;,$$

where the equality follows from $\lambda_x > 0$, which completes the proof of (a). The proof of (b) is a simple calculation and is omitted. We now show (c). If we set $\Lambda'(\epsilon) = 0$, it implies that $\epsilon > 0$ satisfies

$$(1+\lambda_x) - \epsilon R_1^2 = R^{1/2}(\epsilon)(1-\lambda_x) \;, \quad (64)$$

and imposes the condition $(1+\lambda_x) - \epsilon R_1^2 \geq 0$ so

$$\epsilon \in \left[0, \frac{1+\lambda_x}{(1+\lambda_x)^2 + R_0^2}\right] \;. \quad (65)$$

Squaring both sides of (64) implies the following sequence of equalities using (60)

$$(1-\lambda_x)^2 R(\epsilon) = \left[\epsilon R_1^2 - (1+\lambda_x)\right]^2 ,$$
$$(1-\lambda_x)^2 \left[R_1^2\epsilon^2 - 2(1+\lambda_x)\epsilon + 1\right] = R_1^4\epsilon^2 - 2R_1^2(1+\lambda_x)\epsilon + (1+\lambda_x)^2 ,$$

which is equivalent by (62) to

$$R_1^2\epsilon^2\left[(1-\lambda_x)^2 - R_1^2\right] - 2\epsilon(1+\lambda_x)\left[(1-\lambda_x)^2 - R_1^2\right] - 4\lambda_x = 0$$
$$(1+\lambda_x)^2 + R_0^2\epsilon^2\left[-4\lambda_x - R_0^2\right] - 2\epsilon(1+\lambda_x)\left[-4\lambda_x - R_0^2\right] - 4\lambda_x = 0$$
$$((1+\lambda_x)^2 + R_0^2)R_1^2\epsilon^2 - 2(1+\lambda_x)\epsilon + 4\lambda_x/(R_0^2+4\lambda_x) = 0 .$$

The two strictly positive roots are

$$\epsilon_\pm = \frac{(1+\lambda_x) \pm \left[(1+\lambda_x)^2 - 4\lambda_x\{(1+\lambda_x)^2 + R_0^2\}/(R_0^2+4\lambda_x)\right]^{1/2}}{(1+\lambda_x)^2 + R_0^2} > 0,$$

where the inequality follows from $\lambda_x > 0$ and $R_0 > 0$. Further

$$(1+\lambda_x)^2\left(R_0^2+4\lambda_x\right) - 4\lambda_x\left[(1+\lambda_x)^2 + R_0^2\right] = R_0^2\left[(1+\lambda_x)^2 - 4\lambda_x\right] = R_0^2[1-\lambda_x]^2 ,$$

and since $\lambda_x \le 1$, this yields the simplified expression for the two roots

$$\epsilon_\pm = \frac{(1+\lambda_x) \pm (1-\lambda_x)\left[R_0^2/(R_0^2+4\lambda_x)\right]^{1/2}}{(1+\lambda_x)^2 + R_0^2} .$$

From the conditions on ϵ given by (a) and (65), and the fact that $\lambda_x \le 1$, we retain $\epsilon_0 = \epsilon_-$ only. The last statement follows from the second statement and the fact that Λ' is continuous. ☐

The following lemma establishes in particular that ϵ_0 is a global maximum.

Lemma 24. *Let $\Lambda\colon \mathbb{R}_+^* \to \mathbb{R}$ be defined by (21). Then with $\lambda_x \in (0,1)$ and $R_0 > 0$,*

(a) or any $\epsilon > 0$, $\Lambda''(\epsilon) < 0$ (implying concavity),

(b) Λ is maximized at ϵ_0 defined by (63) and $0 < \epsilon_0 \le (4\lambda_x)/(4\lambda_x + R_0^2)$.

(c) If in addition $R_0 \ge 2$, $\epsilon_0 \le 3\lambda_x/(4\lambda_x + R_0^2)$.

Proof. (a) We differentiate $\epsilon \mapsto -2\Lambda(\epsilon) = -[1-\epsilon(1-\lambda_x)] + R^{1/2}(\epsilon)$ twice, yielding the first order derivative

$$\epsilon \mapsto (1-\lambda_x) + (1/2)R'(\epsilon)R^{-1/2}(\epsilon)$$

and the second order derivative follows

$$\epsilon \mapsto (1/2)\left(R''(\epsilon)R^{-1/2}(\epsilon) - (1/2)[R'(\epsilon)]^2R^{-3/2}(\epsilon)\right) = (1/4)R^{-3/2}(\epsilon)\left(2R''(\epsilon)R(\epsilon) - [R'(\epsilon)]^2\right) .$$

Now from (60), $R(\epsilon) = a\psi(\epsilon)$ with $\psi(\epsilon) = (\epsilon-b)^2 + c$ with all constants b, c non-negative. Further $\psi'(\epsilon) = 2(\epsilon - b)$ and $\psi''(\epsilon) = 2$ and therefore

$$2\psi''(\epsilon)\psi(\epsilon) - \psi'(\epsilon)^2 = 4[(\epsilon-b)^2 + c - (\epsilon-b)^2] = 4c > 0 ,$$

which implies that $\Lambda''(\epsilon) \le 0$ for any $\epsilon \ge 0$.

(b) From the concavity we deduce that ϵ_0 is a maximum, and the inequality on ϵ_0 follows from the fact that this is required for $\Lambda(\epsilon_0) \geq 0$.

(c) Using that for any $s \geq 0$, $(1+s)^{1/2} \leq 1 + s/2$, and $4\lambda_x \leq (1+\lambda_x)^2$, we get that

$$\epsilon_0 = R_0 \frac{(1+\lambda_x)(4\lambda_x/R_0^2+1)^{1/2} - (1-\lambda_x)}{\left[(1+\lambda_x)^2 + R_0^2\right](R_0^2+4\lambda_x)^{1/2}} \leq \frac{2\lambda_x R_0 + 2\lambda_x(1+\lambda_x)/R_0}{\left[(1+\lambda_x)^2+R_0^2\right]^{1/2}(R_0^2+4\lambda_x)} \leq \frac{2\lambda_x + 2\lambda_x(1+\lambda_x)/R_0^2}{R_0^2+4\lambda_x} .$$

The assumption $R_0 \geq 2$ completes the proof.

□

Proposition 25. *The function $\tilde{\alpha}\colon \mathbb{R}_+ \to \mathbb{R}_+$, defined by (61), has a unique maximizer $\epsilon^\star \in (0, \epsilon_0)$, where ϵ_0 is given in (63). In addition, if $2^{1/2}R_0 \geq \lambda_v$ then*

$$\tilde{\alpha}(\epsilon_0) \leq \tilde{\alpha}(\epsilon^\star) \leq 3\tilde{\alpha}(\epsilon_0) . \tag{66}$$

Proof. First note that for any $\epsilon \geq 0$,

$$\tilde{\alpha}'(\epsilon) = \frac{\Psi(\epsilon)}{(1+2^{1/2}\lambda_v\epsilon)^2} ,$$

with

$$\Psi(\epsilon) = \Lambda'(\epsilon)(1+2^{1/2}\lambda_v\epsilon) - 2^{1/2}\lambda_v\Lambda(\epsilon) .$$

Then from Lemma 24,

$$\Psi(\epsilon_0) = 2^{1/2}\lambda_v\Lambda(\epsilon_0) < 0 , \qquad \text{and for any } \epsilon \geq 0,\ \Psi'(\epsilon) = (1+2^{1/2}\lambda_v\epsilon)\Lambda''(\epsilon) < 0 . \tag{67}$$

Together with $\Psi(0) = \Lambda'(0) = \lambda_x > 0$, and the fact that $\epsilon \to \Psi(\epsilon)$ is continuous, we deduce the existence and uniqueness of $\epsilon^\star \in (0, \epsilon_0)$ satisfying $\tilde{\alpha}'(\epsilon^\star) = 0$, and maximizing $\tilde{\alpha}$ on $\mathbb{R}_+$. Further since $\tilde{\alpha}'(\epsilon^\star) = 0$ and $\epsilon \mapsto \Psi(\epsilon)$ is non-increasing, using the first equality of (67) and the definition of $\tilde{\alpha}$ given in (61), we deduce

$$\sup_{\epsilon\in[\epsilon^\star,\epsilon_0]} |\tilde{\alpha}'(\epsilon)| \leq \frac{|\Psi(\epsilon_0)|}{(1+2^{1/2}\lambda_v\epsilon^\star)^2} = 2^{1/2}\lambda_v \frac{1+2^{1/2}\lambda_v\epsilon_0}{(1+2^{1/2}\lambda_v\epsilon^\star)^2}\tilde{\alpha}(\epsilon_0) ,$$

From a Taylor's theorem, we obtain

$$\tilde{\alpha}(\epsilon^\star) - \tilde{\alpha}(\epsilon_0) \leq (\epsilon_0 - \epsilon^\star)2^{1/2}\lambda_v \frac{1+2^{1/2}\lambda_v\epsilon_0}{(1+2^{1/2}\lambda_v\epsilon^\star)^2}\tilde{\alpha}(\epsilon_0) ,$$

from which we conclude that

$$\tilde{\alpha}(\epsilon_0) \leq \tilde{\alpha}(\epsilon^\star) \leq \left[1 + (\epsilon_0-\epsilon^\star)2^{1/2}\lambda_v \frac{1+2^{1/2}\lambda_v\epsilon_0}{(1+2^{1/2}\lambda_v\epsilon^\star)^2}\right]\tilde{\alpha}(\epsilon_0) .$$

Now if we use $2^{1/2}R_0 \geq \lambda_v$ we have by (63) that

$$\lambda_v\epsilon_0 < \frac{(1+\lambda_x)\lambda_v}{(1+\lambda_x)^2+R_0^2} \leq \lambda_v(2R_0)^{-1} \leq 2^{-1/2} ,$$

implying

$$(\epsilon_0 - \epsilon^\star) 2^{1/2} \lambda_v \frac{1 + 2^{1/2}\lambda_v \epsilon_0}{(1 + 2^{1/2}\lambda_v \epsilon^\star)^2} \leq 2^{1/2}\lambda_v \epsilon_0 (1 + 2^{1/2}\lambda_v \epsilon_0) \leq 2 ,$$

which completes the proof of (66). ☐

B Some results on closed operators on Hilbert spaces

In this section we gather classical results concerning densely defined closed operators on a Hilbert space to which we repeatedly refer throughout the manuscript.

Proposition 26. *Let $\mathcal{B}$ be a closed and densely defined operator on a Hilbert space H of inner product $\langle \cdot, \cdot \rangle$, induced norm $\|\cdot\|$ and operator norm $|||\cdot|||$.*

(a) $\mathrm{Id} + \mathcal{B}^\star \mathcal{B}$ *is a positive self-adjoint operator on* H *bijective from* $\mathrm{D}(\mathcal{B}^\star\mathcal{B})$ *to* H*. In addition,* $(\mathrm{Id} + \mathcal{B}^\star\mathcal{B})^{-1}$ *is a positive self-adjoint bounded operator on* H *and* $\mathcal{B}(\mathrm{Id} + \mathcal{B}^\star\mathcal{B})^{-1}$ *is a bounded operator.*

(b) For any $h \in \mathsf{H}$,
$$\|(\mathrm{Id} + \mathcal{B}^\star\mathcal{B})^{-1} h\|^2 + 2 \|\mathcal{B}(\mathrm{Id} + \mathcal{B}^\star\mathcal{B})^{-1} h\|^2 \leq \|h\|^2 .$$

(c) $\mathcal{B}^\star\mathcal{B}(\mathrm{Id} + \mathcal{B}^\star\mathcal{B})^{-1}$ *is a bounded operator on* H *which satisfies* $|||\mathcal{B}^\star\mathcal{B}(\mathrm{Id} + \mathcal{B}^\star\mathcal{B})^{-1}||| \leq 1$.

(d) The operator $((\mathrm{Id} + \mathcal{B}^\star\mathcal{B})^{-1}\mathcal{B}^\star, \mathrm{D}(\mathcal{B}^\star))$ *is closable, its closure is a bounded operator and* $|||\overline{(\mathrm{Id} + \mathcal{B}^\star\mathcal{B})^{-1}\mathcal{B}^\star}||| \leq 1$.

Remark 27. *Note that under the condition of Proposition 26, we get that* $(\mathrm{Id} + \mathcal{B}^\star\mathcal{B})^{-1}\mathcal{B}^\star$ *can be extended to a bounded operator and*

$$|||(\mathrm{Id} + \mathcal{B}^\star\mathcal{B})^{-1}||| \leq 1 , \quad |||\mathcal{B}(\mathrm{Id} + \mathcal{B}^\star\mathcal{B})^{-1}||| \leq 1/2^{1/2} .$$

Proof. (a) and (b) follow from [49, Theorem 5.1.9] and inspection of the proof.

We now show (c). First note that $(\mathrm{Id} + \mathcal{B}^\star\mathcal{B} - \mathrm{Id})(\mathrm{Id} + \mathcal{B}^\star\mathcal{B})^{-1} = \mathrm{Id} - (\mathrm{Id} + \mathcal{B}^\star\mathcal{B})^{-1}$, from which we deduce that it is a self-adjoint and bounded operator by the triangle inequality with norm less or equal than 2. To prove the tighter upper bound we use [49, Proposition 3.2.27 p. 99] (twice), the identity for any $h \in \mathsf{H}$

$$\left|\left\langle \mathcal{B}^\star\mathcal{B}(\mathrm{Id} + \mathcal{B}^\star\mathcal{B})^{-1} h, h \right\rangle\right| = \max\left\{ \|h\|^2 - \left\langle (\mathrm{Id} + \mathcal{B}^\star\mathcal{B})^{-1} h, h \right\rangle, \left\langle (\mathrm{Id} + \mathcal{B}^\star\mathcal{B})^{-1} h, h \right\rangle - \|h\|^2 \right\} ,$$

that $(\mathrm{Id} + \mathcal{B}^\star\mathcal{B})^{-1}$ is positive and $|||(\mathrm{Id} + \mathcal{B}^\star\mathcal{B})^{-1}||| \leq 1$ from the first statement.

It remains to prove (d). Since $\mathcal{B}$ is closed and densily defined, $\mathrm{D}(\mathcal{B}^\star)$ is dense and therefore $\{(\mathrm{Id} + \mathcal{B}^\star\mathcal{B})^{-1}\mathcal{B}^\star\}^\star$ is closed and densely defined by [49, Theorem 5.1.5]. By (a), we have for any $h_1 \in \mathrm{D}(\mathcal{B}^\star)$ and $h_2 \in \mathsf{H}$, we have

$$\left\langle (\mathrm{Id} + \mathcal{B}^\star\mathcal{B})^{-1}\mathcal{B}^\star h_1, h_2 \right\rangle_2 = \left\langle h_1, \mathcal{B}(\mathrm{Id} + \mathcal{B}^\star\mathcal{B})^{-1} h_2 \right\rangle_2 ,$$

which implies that $\{(\mathrm{Id} + \mathcal{B}^\star\mathcal{B})^{-1}\mathcal{B}^\star\}^\star = \mathcal{B}(\mathrm{Id} + \mathcal{B}^\star\mathcal{B})^{-1}$. Therefore, $\{(\mathrm{Id} + \mathcal{B}^\star\mathcal{B})^{-1}\mathcal{B}^\star\}^{\star\star}$ is a bounded operator on H. The proof then follows by [49, Theorem 5.1.5] which implies that $(\mathrm{Id} + \mathcal{B}^\star\mathcal{B})^{-1}\mathcal{B}^\star$ is closable and $\overline{(\mathrm{Id} + \mathcal{B}^\star\mathcal{B})^{-1}\mathcal{B}^\star} = ((\mathrm{Id} + \mathcal{B}^\star\mathcal{B})^{-1}\mathcal{B}^\star)^{\star\star}$. ☐

A similar result can be obtained by using that $\mathcal{B}$ is closable only, as a consequence of the following lemma.

Lemma 28. *Assume that $(\mathcal{B}, \mathrm{D}(\mathcal{B}))$ is a densely defined closable operator. Let $(\overline{\mathcal{B}}, \mathrm{D}(\overline{\mathcal{B}}))$ be the closure of $(\mathcal{B}, \mathrm{D}(\mathcal{B}))$ and $m > 0$. Then, the conclusions of Proposition 26 hold changing $\mathcal{B}$ to $\overline{\mathcal{B}}$.*

Proof. This result is a just a consequence of [49, Theorem 5.1.5] which implies that $\mathcal{B}^\star$ is densely defined, $\overline{\mathcal{B}} = (\mathcal{B}^\star)^\star$ and $\mathcal{B}^\star = \overline{\mathcal{B}}^\star$. □

The densely defined and closed operator ∇_x on $\mathrm{L}^2(\pi)$ can be extended as an operator on $\mathrm{L}^2(\pi)^d$ as follows: for any $(f_1, \ldots, f_d) \in \mathrm{L}^2(\pi)^d$, $f_1 \in \mathrm{D}(\nabla_x)$, $\nabla_x f = \nabla_x f_1$. Therefore a direct consequence of Proposition 26 applied to the operator $m^{-1/2}\nabla_x$ for $m > 0$, on $\mathrm{L}^2(\pi)^d$ is the following.

Corollary 29. *Let $m > 0$. The operators $\nabla_x(m \operatorname{Id} + \nabla_x^\star \nabla_x)^{-1}$ and $\nabla_x^\star \nabla_x (m \operatorname{Id} + \nabla_x^\star \nabla_x)^{-1}$ are bounded on $\mathrm{L}^2(\pi)^d$ with*

$$\left\| \nabla_x (m \operatorname{Id} + \nabla_x^\star \nabla_x)^{-1} \right\|_{\mathrm{L}^2(\pi)} \leq 1/(2m)^{1/2} \ , \ \left\| \nabla_x^\star \nabla_x (m \operatorname{Id} + \nabla_x^\star \nabla_x)^{-1} \right\|_{\mathrm{L}^2(\pi)} \leq 1 \ .$$

In addition, for any $f \in \mathrm{L}^2(\pi)$,

$$\left\| (m \operatorname{Id} + \nabla_x^\star \nabla_x)^{-1} f \right\|_2^2 + (2/m) \left\| \nabla_x (m \operatorname{Id} + \nabla_x^\star \nabla_x)^{-1} f \right\|_2^2 \leq \{ \|f\|_2 / m \}^2 \ ,$$

and

$$\left\| \nabla_x^\star \nabla_x (m \operatorname{Id} + \nabla_x^\star \nabla_x)^{-1} f \right\|_2 \leq \|f\|_2 \ .$$

We conclude this section by the following results which can be found in [31].

Lemma 30 ([31, Lemma 2.2])**.** *Let $(\mathcal{T}, \mathrm{D}(\mathcal{T}))$ be a anti-symmetric operator on $\mathrm{L}^2(\mu)$ and Π be an orthogonal projection on $\mathrm{L}^2(\mu)$. Assume that there exists $\mathsf{D} \subset \mathrm{D}(\mathcal{T})$ such that $\Pi(\mathsf{D}) \subset \mathrm{D}(\mathcal{T})$ and D is dense in $\mathrm{L}^2(\mu)$. Then the following statements hold.*

(a) $\mathrm{D}(\mathcal{T}) \subset \mathrm{D}((\mathcal{T}\Pi)^\star)$ and for any $f \in \mathrm{D}(\mathcal{T})$, $(\mathcal{T}\Pi)^\star f = -\Pi \mathcal{T} f$.

(b) For any $f \in \mathrm{D}((\mathcal{T}\Pi)^\star)$, $\Pi(\mathcal{T}\Pi)^\star f = (\mathcal{T}\Pi)^\star f$.

C Elliptic regularity estimates

We preface this section with some complements on the adjoint of ∇_x seen as an operator on $\mathrm{L}^2(\pi)^d$.

Lemma 31. *Assume **H**1. Consider the operator $(\nabla_x, \mathrm{D}(\nabla_x))$ from the Hilbert space $\mathrm{L}^2(\pi)$ to $\mathrm{L}^2(\pi)^d$ endowed with the inner product defined by (5). Then it holds*

(a) for any $i \in \{1, \ldots, d\}$, the $\mathrm{L}^2(\pi)$-adjoint of ∂_{x_i} is given for any $g \in \mathrm{C}^1_{\mathrm{poly}}(\mathsf{X})$ by

$$\partial_{x_i}^\star g = -\partial_{x_i} g + g \partial_{x_i} U \ ;$$

(b) the $\mathrm{L}^2(\pi)$-adjoint of ∇_x is given for any $G \in \mathrm{C}^1_{\mathrm{poly}}(\mathsf{X}, \mathbb{R}^d)$ by

$$\nabla_x^\star G = -\operatorname{div}_x G + \nabla_x U^\top G \ .$$

Remark 32. *Note that Lemma 31 implies that for any* $g \in \mathrm{C}^2_{\mathrm{poly}}(\mathsf{X})$ *and* $G \in \mathrm{C}^2_{\mathrm{poly}}(\mathsf{X}, \mathbb{R}^d)$*, we have*

$$\nabla_x^\star \nabla_x g = -\Delta_x g + \nabla_x U^\top \nabla_x g \text{ and } \nabla_x \nabla_x^\star G = \nabla_x^\star \nabla_x G + \nabla_x^2 U G \,, \tag{68}$$

where we have defined $\nabla_x^\star \nabla_x G \in \mathrm{C}_{\mathrm{poly}}(\mathsf{E}, \mathbb{R}^d)$ *for any* $(x, v) \in \mathsf{E}$ *and* $i \in \{1, \ldots, d\}$ *by*

$$\{\nabla_x^\star \nabla_x G(x, v)\}_i = \nabla_x^\star \partial_{x_i} G(x, v) = \sum_{j=1}^d -\partial_{x_j, x_i} G_j(x, v) + \partial_{x_j} U(x) \partial_{x_i} G(x, v) \,.$$

Proof. The proof just follows by integration by parts. □

Proposition 33. *Let* $m > 0$ *and assume* ***H**1. Then for any* $f \in \mathrm{C}^2_{\mathrm{b}}(\mathsf{E})$*,*

$$\|\nabla_x^2 (m \operatorname{Id} + \nabla_x^\star \nabla_x)^{-1} \Pi_v f\|_2 \leq \kappa_1 \|\Pi_v f\|_2 \quad \text{where} \quad \kappa_1 = (1 + c_1/(2m))^{1/2} \,. \tag{69}$$

Proof. Let $f \in \mathrm{C}^2_{\mathrm{b}}(\mathsf{E})$ and consider $u = (m \operatorname{Id} + \nabla_x^\star \nabla_x)^{-1} \Pi_v f$. By [48, Theorem 2], $u \in \mathrm{C}^3_{\mathrm{poly}}(\mathsf{X})$. Therefore we obtain by (68), (10) and the fact that $U \in \mathrm{C}^3_{\mathrm{poly}}(\mathsf{X})$ using **H**1,

$$\begin{aligned} \|\nabla_x^2 u\|_2^2 = \langle \nabla_x^2 u, \nabla_x^2 u \rangle_2 = \langle \nabla_x u, (\nabla_x^\star \nabla_x)[\nabla_x u] \rangle_2 &= \langle \nabla_x u, (\nabla_x \nabla_x^\star)[\nabla_x u] - \nabla_x^2 U \nabla_x u \rangle_2 \\ &= \|\nabla_x^\star \nabla_x u\|_2^2 - \langle \nabla_x u, \nabla_x^2 U \nabla_x u \rangle_2 \,. \end{aligned} \tag{70}$$

From the definition of u, using Corollary 29 and **H**1-(a) we conclude that

$$\|\nabla_x^2 u\|_2^2 \leq \|\Pi_v f\|_2^2 + c_1 \|\nabla_x u\|_2^2 \leq \|f\|_2^2 + c_1 \|\Pi_v f\|_2^2 / (2m) \,.$$

□

In order to bound terms of the form $\|F_k^\top \nabla_x u\|$ in Section 3.3 we need the following Lemma which is a quantitative version of [21, Lemma 6]. Consider the function $W : \mathbb{R}^d \to \mathbb{R}_+$ defined for any $x \in \mathbb{R}^d$ by

$$W(x) = \left\{1 + |\nabla_x U(x)|^2\right\}^{1/2} \,. \tag{71}$$

Lemma 34 ([21, Lemma 6])**.** *Assume* ***H**1. Then for any* $\varphi \in \mathrm{D}(\nabla_x)$*,*

$$\|\nabla_x \varphi\|_2 \geq \left[4\left(1 + c_2 d^{1+\varpi}/(4C_{\mathrm{P}}^2)\right)^{1/2}\right]^{-1} \|\varphi \nabla_x U\|_2 \,,$$

where c_2 *and* C_{P} *are defined in (9) and (8) respectively. As a corollary, it holds for any* $\varphi \in \mathrm{D}(\nabla_x)$*,*

$$\begin{aligned} \|\nabla_x \varphi\|_2 \geq \kappa_2 \|\varphi W\|_2 \text{ , where } \kappa_2^{-1} &= \left(C_{\mathrm{P}}^{-2} + 16(1 + c_2 d^{1+\varpi}/(4C_{\mathrm{P}}^2))\right)^{1/2} \\ &= C_{\mathrm{P}}^{-1}\left(1 + 4c_2 d^{1+\varpi} + 16 C_{\mathrm{P}}^2\right)^{1/2} \geq C_{\mathrm{P}}^{-1} \,. \end{aligned} \tag{72}$$

Proof. Note that we only need to consider $\varphi \in \mathrm{C}^\infty_{\mathrm{c}}(\mathsf{X})$ since $\mathrm{C}^\infty_{\mathrm{c}}(\mathsf{X})$ is a core for $(\nabla_x, \mathrm{D}(\nabla_x))$. First since $\nabla_x U \in \mathrm{L}^2(\mu)$, for any $\varepsilon > 0$, we get

$$2 \langle \varphi \nabla_x U, \nabla_x \varphi \rangle_2 \leq \varepsilon^{-1} \|\nabla_x \varphi\|_2^2 + \varepsilon \|\varphi \nabla_x U\|_2^2 \,. \tag{73}$$

We then bound from below the left-hand side. Using the *carré du champ* identity, *i.e.* for any $f, g \in \mathrm{C}^2_{\mathrm{poly}}(\mathsf{X})$, $\langle \nabla_x f, \nabla_x g\rangle_2 = \left\langle \nabla_x U^\top \nabla_x f - \Delta_x f, g\right\rangle_2$, we get using that $\nabla_x[\varphi^2] = 2\varphi\nabla_x\varphi$,

$$2\left\langle \varphi\nabla_x U, \nabla_x\varphi\right\rangle_2 = \left\langle \nabla_x[\varphi^2], \nabla_x U\right\rangle_2 = \|\varphi\nabla_x U\|_2^2 - \left\langle \varphi^2, \Delta_x U\right\rangle_2 \ .$$

By (9) and (8), we obtain

$$2\left\langle \varphi\nabla_x U, \nabla_x\varphi\right\rangle_2 \geq \|\varphi\nabla_x U\|_2^2/2 - c_2 d^{1+\varpi}\|\varphi\|_2^2 \geq \|\varphi\nabla_x U\|_2^2/2 - (c_2 d^{1+\varpi}/C_{\mathrm{P}}^2)\|\nabla_x\varphi\|_2^2 \ .$$

From this result and (73), it follows that

$$\|\varphi\nabla_x U\|_2^2/2 - (c_2 d^{1+\varpi}/C_{\mathrm{P}}^2)\|\nabla_x\varphi\|_2^2 \leq \varepsilon^{-1}\|\nabla_x\varphi\|_2^2 + \varepsilon\|\varphi\nabla_x U\|_2^2 \ .$$

Rearranging terms and setting $\varepsilon = 1/4$ completes the proof. The last statement is a direct consequence of the first one using the definition of W in (71). □

Putting this with Proposition 33, this implies the following.

Corollary 35. *Let $m > 0$ and assume **H**1 and **H**2. For any $f \in \mathrm{L}^2(\mu)$ and $k \in \{1, \ldots, K\}$, we have*

$$\left\|F_k^\top\{\nabla_x(m\,\mathrm{Id} + \nabla_x^\star\nabla_x)^{-1}\Pi_v f\}\right\|_2 \leq 2^{1/2}a_k\left\|W\{\nabla_x(m\,\mathrm{Id} + \nabla_x^\star\nabla_x)^{-1}\Pi_v f\}\right\|_2 \leq \frac{2^{1/2}a_k\kappa_1}{\kappa_2}\|\Pi_v f\|_2 \ ,$$

where a_k, W, κ_1 and κ_2 are defined by (11), (71), (69) and (72) respectively.

Proof. Note first that since $\nabla_x(m\,\mathrm{Id} + \nabla_x^\star\nabla_x)^{-1}$ is a bounded operator by Corollary 29, it is sufficient by density to show this result for $f \in \mathrm{C}^2_{\mathrm{b}}(\mathsf{E})$. Let $f \in \mathrm{C}^2_{\mathrm{b}}(\mathsf{E})$ and $u = (m + \nabla_x^\star\nabla_x)^{-1}\Pi_v f$. By [48, Theorem 2], $u \in \mathrm{C}^3_{\mathrm{poly}}(\mathsf{X})$. Second since for any $t, s \geq 0$, $s + t \leq 2^{1/2}\sqrt{s^2 + t^2}$, **H**2-(c) implies for any $x \in \mathsf{X}$,

$$|F_k|(x) \leq a_k(1 + |\nabla_x U|(x)) \leq 2^{1/2}a_k W(x) \ .$$

Therefore using Lemma 34 and Proposition 33 successively, we obtain

$$\begin{aligned}\left\|F_k^\top\nabla_x u\right\|_2 &\leq \|\,|F_k|\,\nabla_x u\,\|_2 \leq 2^{1/2}a_k\|W\nabla_x u\|_2 = 2^{1/2}a_k\left(\sum_{i=1}^d\|W\partial_{x_i}u\|_2^2\right)^{1/2} \\ &\leq (2^{1/2}a_k/\kappa_2)\left(\sum_{i=1}^d\|\nabla_x[\partial_{x_i}u]\|_2^2\right)^{1/2} = (2^{1/2}a_k/\kappa_2)\left\|\nabla_x^2 u\right\|_2 \leq (2^{1/2}a_k\kappa_1/\kappa_2)\|\Pi_v f\|_2 \ .\end{aligned}$$

□

D Radial distributions

The following gathers standard results on spherically symmetric distributions on $\mathbb{R}^d$ for which we could not find a single reference. In particular we establish that **H**4-(a) and conditions required in Lemma 38 are satisfied in this scenario.

Lemma 36. *Let $d \geq 2$.*

(a) *Assume ν is the uniform distribution on the unit hypersphere $\mathbb{S}^{d-1}$, then*

(i) *for $i,j,k,l \in \{1,\dots,d\}$ such that* $\mathrm{card}(\{i,j,k,l\}) > 2$*, we have* $\int_{\mathbb{S}^{d-1}} v_i v_j v_k v_l \,\mathrm{d}\nu(v) = 0$*,*

(ii) *otherwise,*

$$m_2 = \frac{1}{d}\,, \qquad m_{2,2} = \int_{\mathbb{S}^{d-1}} v_1^2 v_2^2 \,\mathrm{d}\nu(v) = \frac{1}{d(d+2)} \text{ and } \qquad m_4 = \frac{1}{3}\int_{\mathbb{S}^{d-1}} v_1^4 \,\mathrm{d}\nu(v) = \frac{1}{d(d+2)}\,.$$

(b) *For any spherically symmetric distribution ν i.e. corresponding to random variables $V = B^{1/2}W$ for W uniformly distributed on the unit hypersphere $\mathbb{S}^{d-1}$ and B a non-negative random variable independent of w and of first and second order moments γ_1 and γ_2 respectively,*

(i) *for $i,j,k,l \in \{1,\dots,d\}$ such that* $\mathrm{card}(\{i,j,k,l\}) > 2$*, we have* $\int_{\mathbb{R}^d} v_i v_j v_k v_l \,\mathrm{d}\nu(v) = 0$*,*

(ii) *otherwise,*

$$m_2 = \frac{\gamma_1}{d}\,, \qquad m_{2,2} = \frac{\gamma_2}{d(d+2)} \text{ and } \qquad m_4 = \frac{\gamma_2}{d(d+2)}\,.$$

Remark 37. *Naturally the zero-mean d-dimensional Gaussian distribution on $\mathbb{R}^d$ with covariance matrix* I_d*. corresponds to B distributed according to $\chi^2(d)$, in which case $m_4 = m_{2,2} = m_2^2$.*

Proof. We use the polar parametrization of the multivariate normal distribution. Let

$$v(\phi) = \big(\cos\phi_1, \sin\phi_1\cos\phi_2, \dots, \cos(\phi_k)\prod_{i=1}^{k-1}\sin(\phi_i), \dots, \prod_{i=1}^{d-1}\sin(\phi_i)\big),$$

$\phi \in [0,\pi]^{d-2} \times [0,2\pi]$. The probability distribution for ϕ ensuring uniformity of $v(\phi)$ on the surface of the d-sphere has density

$$f_{\mathbb{S}}(\phi) \propto \prod_{i=1}^{d-2} \sin^{d-i-1}(\phi_i)\mathbb{1}_{[0,\pi]^{d-2}\times[0,2\pi]}(\phi)\,,$$

with respect to the Lebesgue measure on $\mathbb{R}^{d-1}$. Let Φ be random variable with distribution $f_{\mathbb{S}}$. Further let $B \sim \chi^2(d)$ be independent of Φ then it is standard knowledge that $W = B^{1/2}v(\Phi)$ follows the zero-mean d-dimensional Gaussian distribution on $\mathbb{R}^d$ with covariance matrix I_d. Therefore, by construction,

$$\begin{aligned}\mathbb{E}\big[W_iW_jW_kW_l\big] = \mathbb{E}\big[B^2 v_i(\Phi)v_j(\Phi)v_k(\Phi)v_l(\Phi)\big] &= \mathbb{E}\big[B^2\big]\mathbb{E}\big[v_i(\Phi)v_j(\Phi)v_k(\Phi)v_l(\Phi)\big] \\ &= d(d+2)\mathbb{E}\big[v_i(\Phi)v_j(\Phi)v_k(\Phi)v_l(\Phi)\big]\,,\end{aligned}$$

and the latter term vanishes when the leftmost term does. We also deduce that

$$\mathbb{E}\big[W_1^2\big]\mathbb{E}\big[W_2^2\big] = \mathbb{E}\big[W_1^2W_2^2\big] = d(d+2)\mathbb{E}\big[v_1^2(\Phi)v_2^2(\Phi)\big]\,,$$

from which we obtain $\mathbb{E}\big[v_1^2(\Phi)v_2^2(\Phi)\big]$. Similarly using properties of the moments of the normal distribution,

$$3\mathbb{E}\big[W_1^2\big]^2 = \mathbb{E}\big[W_1^4\big] = d(d+2)\mathbb{E}\big[v_1^4(\Phi)\big]\,,$$

leading to the expression for $\mathbb{E}\big[v_1^4(\Phi)\big]$. The last statement is straightforward.

□

E Expectation of quadratic forms of the velocity

This section provides expressions for second order moments of quadratic forms of v for a large class of distributions for which we could not find adequate references.

Lemma 38. *Let $M \in \mathbb{R}^{d\times d}$ be a symmetric matrix, $c \in \mathbb{R}$ and assume the distribution ν of v is such that*

(a) for any bounded and measurable function $f : \mathbb{R}^2 \to \mathbb{R}$, $i, j \in \{1, \dots, d\}$ such that $i \neq j$, $\int f(v_i, v_j)\,\mathrm{d}\nu(v) = \int f(v_1, v_2)\,\mathrm{d}\nu(v)$

(b) for $i, j, k, l \in \{1, \dots, d\}$, we have $\int v_i v_j v_k v_l \,\mathrm{d}\nu(v) = 0$ whenever $\operatorname{card}(\{i, j, k, l\}) > 2$.

Then

$$\left\|v^\top M v - c\right\|_\nu^2 = 3(m_4 - m_{2,2})\mathrm{Tr}(M \odot M) + (m_2 \mathrm{Tr}(M) - c)^2 + 2m_{2,2}\mathrm{Tr}(M^2),$$

where $\odot$ denotes the Hadamard product.

Proof. Using that M is symmetric, and the expectation symbol for expectations with respect to ν,

$$\mathbb{E}\left[\left(\sum_{i,j=1}^d M_{ij} v_i v_j - c\right)^2\right] = \sum_{i,j,k,\ell=1}^d M_{ij} M_{k\ell} \mathbb{E}[v_i v_j v_k v_\ell] - 2c \sum_{i,j=1}^d M_{ij} \mathbb{E}[v_i v_j] + c^2$$

where

$$\begin{aligned}
\sum_{i,j,k,\ell=1}^d M_{ij} M_{k\ell} \mathbb{E}[v_i v_j v_k v_\ell] &= 3m_4 \sum_{i=1}^d M_{ii}^2 + m_{2,2} \sum_{i\neq j} M_{ii} M_{jj} + 2m_{2,2} \sum_{i \neq j} M_{ij}^2 \\
&= (3m_4 - 3m_{2,2}) \sum_{i=1}^d M_{ii}^2 + m_{2,2} \sum_{i,j=1}^d \left(M_{ii} M_{jj} + 2M_{ij}^2\right) \\
&= (3m_4 - 3m_{2,2})\mathrm{Tr}(M \odot M) + m_{2,2}\left(\mathrm{Tr}(M)^2 + 2\mathrm{Tr}(M^2)\right).
\end{aligned}$$

Therefore

$$\begin{aligned}
\mathbb{E}\left[\left(\sum_{i,j=1}^d M_{ij} v_i v_j - c\right)^2\right] &= (3m_4 - 3m_{2,2})\mathrm{Tr}(M \odot M) + m_{2,2}\mathrm{Tr}(M)^2 + 2m_{2,2}\mathrm{Tr}(M^2) \\
&\quad - 2cm_2 \mathrm{Tr}(M) + c^2,
\end{aligned}$$

which implies the desired result. □

Corollary 39. *Given a symmetric matrix $M \in \mathbb{R}^{d\times d}$ and a constant $c \in \mathbb{R}$,*

$$\left\|v^\top M v - m_2 \mathrm{Tr}(M)\right\|_\nu \leq \sqrt{2m_{2,2} + 3(m_4 - m_{2,2})_+}|M|.$$

F Examples of potentials

Lemma 40. *Assume that the potential U is defined for any $x \in \mathsf{X}$ by $U(x) = \sum_{i=1}^d \left(1 + x_i^2\right)^\beta / 2$, for $\beta \geq 1$. Then U is strongly convex and there exists $c_2 > 0$, dependent on β only, such that (9) is satisfied with $\varpi = 0$.*

Proof. We have for $i, j \in \{1, \ldots, d\}$ and $x \in \mathsf{X}$,

$$\left[\nabla_x U(x)\right]_i = \beta x_i \left(1 + x_i^2\right)^{\beta-1} \text{ and } \left[\nabla_x^2 U(x)\right]_{i,j} = \beta[1 + (2\beta - 1)x_i^2]\left(1 + x_i^2\right)^{\beta-2} \delta_{i,j} ,$$

leading to $\nabla_x^2 U(x) \succeq \beta \, \mathrm{I}_d$, and the strong convexity follows. Using that $\beta \geq 1$ and for any $s \geq 0$ and $c > 0$, $(1 + s^2)^{\beta-2} s^2 \leq (1 + c^2)^{\beta-2} c^2 \mathbb{1}_{[0,c]}(s) + (1 + s^2)^{2\beta-2} s^2 / (1 + c^2)^\beta \mathbb{1}_{(c,+\infty)}(s)$ and $(1 + s^2)^{\beta-2} \leq \{1 \vee (1 + c^2)^{\beta-2}\} \mathbb{1}_{[0,c]}(s) + (1 + s^2)^{2\beta-2} (s/c)^2 \mathbb{1}_{(c,+\infty)}(s)$, we get for any $x \in \mathsf{X}$,

$$\begin{aligned}
&\Delta_x U(x) = \mathrm{Tr}(\nabla_x^2 U(x)) = \beta \sum_{i=1}^d [1 + (2\beta - 1)x_i^2]\left(1 + x_i^2\right)^{\beta-2} \\
&\leq \beta d \left[\{1 \vee (1 + c^2)^{\beta-2}\} + (2\beta - 1)(1 + c^2)^{\beta-2} c^2\right] + \beta^{-1} \left|\nabla_x U(x)\right|^2 \left[c^{-2} + (2\beta - 1)(1 + c^2)^{-\beta}\right] ,
\end{aligned}$$

which with $c \geq (2\beta^{-1/2}) \vee 2^{1/\beta}$ completes the proof. □

Lemma 41. *Assume that the potential U is defined for any $x \in \mathsf{X}$ by $U(x) = (1 + |x|^2)^\beta$ with $\beta \geq 1$. Then U is strongly convex and there exists $c_2 > 0$, dependent on β only, such that (9) is satisfied with $\varpi = 1 - 1/\beta$.*

Proof. First, we have that

$$\nabla_x U(x) = 2\beta(1 + |x|^2)^{\beta-1} x = 2\beta U(x)^{1-1/\beta} x, \tag{74}$$

and

$$\nabla_x^2 U(x) = 2\beta \left[(1 - 1/\beta) U^{-1/\beta}(x) \nabla_x U(x) x^\top + U^{1-1/\beta}(x) \, \mathrm{I}_d\right] . \tag{75}$$

As a result, and since $\beta \geq 1$,

$$(1 - \beta^{-1}) U^{-1/\beta}(x) \nabla_x U(x) x^\top = 2\beta U(x)^{1-2/\beta} x x^\top \succeq 0, \qquad , U^{1-1/\beta}(x) I \succeq \mathrm{I}_d ,$$

from which we conclude that for any $x \in \mathsf{X}$, $\nabla_x^2 U(x) \succeq 2\beta \, \mathrm{I}_d$. It remains to show that (9) holds. First we have for any $x \in \mathsf{X}$,

$$\begin{aligned}
\mathrm{Tr}\left(\nabla_x^2 U(x)\right) &= 2(\beta - 1) U^{-1/\beta}(x) x^\top \nabla_x U(x) + 2\beta d \, U^{1-1/\beta}(x) \\
&\leq 2(\beta - 1)|\nabla_x U(x)| \frac{|x|}{1 + |x|^2} + 2\beta d \, U^{1-1/\beta}(x) .
\end{aligned}$$

Using that for any $s \geq 0$ and $a > 0$, $2s \leq a^{-2} + (as)^2$, $(1+s^2)^{\beta-1} \leq (1+(2d/\beta)^{1/\beta})^{\beta-1} \mathbb{1}_{[0,(2d/\beta)^{1/\beta}]}(s^2) + (2d/\beta)^{-1} s^{2\beta} (1 + s^2)^{\beta-1} \mathbb{1}_{((2d/\beta)^{1/\beta},+\infty)}(s^2) \leq (1 + (2d/\beta)^{1/\beta})^{\beta-1} \mathbb{1}_{[0,(2d/\beta)^{1/\beta}]}(s^2) + (2d/\beta)^{-1} s^2 (1 +$

$s^2)^{2\beta-2}\mathbb{1}_{((2d/\beta)^{1/\beta},+\infty)}(s^2)$, (74)-(75), we get for any $x \in \mathsf{X}$,

$$\begin{aligned}\operatorname{Tr}\left(\nabla_x^2 U(x)\right) &\leq 2(\beta-1)|\nabla_x U(x)||x|(1+|x|^2)^{-1} + 2\beta d\, U^{1-1/\beta}(x) \\ &\leq (\beta-1)(4\beta + |\nabla_x U(x)|^2/(4\beta)) + 2\beta d[(1+(2d/\beta)^{1/\beta})^{\beta-1} + |\nabla_x U(x)|^2/(8d\beta)] \\ &\leq 4(\beta-1)\beta + 2^{\beta-1}\beta d(1+(2d/\beta)^{1-1/\beta}) + |\nabla_x U(x)|^2/2\,,\end{aligned}$$

where we used in the last step which completes the proof, that $(a+b)^{\beta-1} \leq 2^{\beta-2}(a^{\beta-1}+b^{\beta-1})$ for any $a, b \geq 0$, applying Hölder inequality, since $\beta \geq 1$. ◻

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