A UNIFYING AND CANONICAL DESCRIPTION OF
MEASURE-PRESERVING DIFFUSIONS

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Abstract. A complete recipe of measure-preserving diffusions in Euclidean
space was recently derived unifying several MCMC algorithms into a single
framework. In this paper, we develop a geometric theory that improves and
generalises this construction to any manifold. We thereby demonstrate that the
completeness result is a direct consequence of the topology of the underlying
manifold and the geometry induced by the target measure \(P\); there is no need
to introduce other structures such as a Riemannian metric, local coordinates,
or a reference measure. Instead, our framework relies on the intrinsic geometry
of \(P\) and in particular its canonical derivative, the deRham rotationnel, which
allows us to parametrise the Fokker–Planck currents of measure-preserving
diffusions using potentials. The geometric formalism can easily incorporate
constraints and symmetries, and deliver new important insights, for example,
a new complete recipe of Langevin-like diffusions that are suited to the
construction of samplers. We also analyse the reversibility and dissipative
properties of the diffusions, the associated deterministic flow on the space of
measures, and the geometry of Langevin processes. Our article connects ideas
from various literature and frames the theory of measure-preserving diffusions
in its appropriate mathematical context.

Keywords. MCMC, Hamiltonian Monte Carlo, Measure-preserving Diffu-
sions, Geometric Statistics, Langevin Processes

1. Introduction

Markov processes play a prominent role in many areas of science. In particular,
continuous diffusion processes that are designed to preserve a given target mea-
ure \(P\) underpin numerous important algorithms. For instance in physics, many
models rely on stochastic Hamiltonian dynamics in which mechanical systems are
coupled to a fluctuating thermostat process preserving the Boltzmann–Gibbs dis-
tribution, see [144, 156]. These processes have also inspired various deep learning
and optimisation methods [43, 59, 66, 113, 150, 162], as well as sampling algo-
rithms to approximate expectations of observables by generating a Markov chain
\((X_i)\) composed of \(P\)-preserving transition kernels,

\[
\mathbb{E}_P[f] = \int f dP \approx \frac{1}{\ell} \sum_i f(X_i),
\]

see [28, 35, 78, 107, 153]. These include Hamiltonian Monte Carlo (HMC) samplers
which originated in lattice QCD [42, 50, 155], and have, since then, been widely
applied from chemistry to statistics [11, 15, 23, 68, 92, 112, 133, 160, 120]. Measure-preserving diffusions are also used to construct Stein operators via the
generator approach [11, 12], with applications to inference, goodness-of-fit tests, measuring sample qualities and approximating distributions [16, 38, 70, 71, 116].

A crucial prerequisite among these applications is the ability for practitioners to construct tailored measure-preserving diffusions; hence the need for a general characterisation and recipe to construct them. In Euclidean space, such a recipe was recently derived in [121], extending previous results including [87, 145, 151, 163]. More precisely, they proved that any continuous Markov process preserving a target measure of the form \( P \propto e^{-H} \, dx \) and satisfying an integrability assumption can be expressed as

\[
\begin{align*}
\frac{dZ_t}{dt} &= - (Q \nabla H + D \nabla H) \, dt + \nabla \cdot (Q + D) \, dt + \sqrt{2D} \, dW_t,
\end{align*}
\]

where \( Q \) and \( D \) are antisymmetric and positive semi-definite position-dependent matrices respectively.

However, this recipe suffers from several important drawbacks preventing its use in some modern applications, in particular:

**Theoretical:** From a theoretical viewpoint, the target distribution in [121] is specified with respect to the Lebesgue measure in Cartesian coordinates, and is thus inappropriate when other coordinates or reference measures are used. Moreover, it cannot easily incorporate geometric properties such as symmetries or conserved quantities that require a geometric framework. In addition, the derivation in [121] relies on an ad hoc construction of \( Q \) based on Fourier transforms, which cannot be generalised to arbitrary manifolds and requires an additional integrability assumption. Instead, we wish to obtain a deeper understanding of the reason why \( P \)-preserving diffusions must take the form (1). Ideally, the construction should solely depend on the target measure \( P \), as this is the only object generally given in applications, and should properly incorporate the assumption that \( P \) is a smooth distribution.

**Practical:** From the viewpoint of applications, the restriction of the recipe to Euclidean spaces dramatically restricts its scope, as many modern applications require \( P \)-preserving diffusions on manifolds. These include thermodynamic integration, free energy calculation and molecular simulations [106, 109, 111, 153], spectral density estimation of partially observed models for Bayesian methods, directional statistics, and lattice QCD calculations on compact Lie groups [17, 33, 34, 47, 72, 80, 81, 115, 126, 164], as well as applications that are built using Stein operators on manifolds, diffusions on spaces with symmetries used in robotics (such as coupled rigid body motion), or for learning to encode symmetries in neural nets [18, 41, 91, 102, 114].

**Main contributions and Structure of the Paper.** In this article, we derive the characterisation of \( P \)-preserving diffusions for any smooth positive measure \( P \) on an arbitrary \( n \)-dimensional manifold \( M \), thus solving this problem in complete generality. Just as importantly, we derive connections with other fields such as Poisson geometry, thermodynamics, and cohomology that explains how the construction fits in the bigger picture of mathematics. By leveraging the geometry generated by \( P \), we provide a canonical construction for these diffusions, without introducing any other structures on \( M \), such as coordinates, a connection, a reference measure, a metric, or other mechanical structures like a Poisson bi-vector field.
Following the ideas from de Rham and Koszul, we rely on the \( P \)-musical isomorphisms \( P^\flat \) and \( P^\sharp \) between multi-vector fields and twisted differential forms to construct the \( P \)-rotationnel \( \text{curl}_P \equiv P^\flat \circ d \circ P^\flat \) (introduced in 3), which transforms the calculus of twisted differential forms associated to the exterior derivative \( d \) into a measure-informed calculus of multi-vector fields associated to \( \text{curl}_P \). The operators \( P^\flat \) and \( \text{curl}_P \) induce the canonical geometry of the target \( P \), which can then be used to show that any \( P \)-preserving diffusion on any manifold takes the form

\[
\begin{aligned}
\frac{d}{dt} Z_t &= \text{Fokker-Planck potential} + \text{topological obstruction} + \text{\( L^2(P) \)-symmetric fluctuation-dissipation balance} \\
&= \text{conservative } L^2(P) \text{-antisymmetric} + \text{dissipative drift} + \text{Stratonovich noise}
\end{aligned}
\]

Here, the conservative term \( \text{curl}_P(\mathcal{A}) + P^\sharp(\gamma) \) characterises the set of all \( P \)-preserving vector fields. Indeed, by analogy with the construction of the magnetic vector potential in physics, we can locally build for any \( P \)-preserving vector field \( X \), a ‘bi-vector potential’ \( \mathcal{A} \) such that \( X = \text{curl}_P(\mathcal{A}) \). We will see that globally, this holds up to topological obstructions, which is represented by the term \( P^\sharp(\gamma) \), where \( \gamma \) is a representative of the \((n-1)\)-twisted de Rham cohomology group. In addition to this, the dissipative term \( \text{div}_P(Y_i)Y_i \) balances the fluctuations introduced by the arbitrary noise process \( Y_i \circ dW^i_t \), as in the fluctuation-dissipation theorem of statistical physics, ensuring that the stochastic and dissipative components of (2), when combined, are also \( P \)-preserving.

Furthermore, when the target \( P \) is expressed as \( P = e^{-H} \mu_M \), where \( \mu_M \) is an arbitrary smooth positive reference measure on \( M \), equation (2) can be decomposed as follows:

\[
\begin{aligned}
\frac{d}{dt} Z_t &= \text{local potential of Fokker-Planck current} + \text{topological obstruction} \\
&= \text{volume-preserving} + \text{density-preserving} + \text{\( L^2(P) \)-symmetric fluctuation-dissipation balance} \\
&= \text{conservative } L^2(P) \text{-antisymmetric drift} + \text{density-dissipative drift} + \text{volume-dissipative drift} + \text{Stratonovich noise}
\end{aligned}
\]

where \( X^\mathcal{A}_H \equiv \mathcal{A}(dH, \cdot) \) is a vector field generated by the log-density \( H \), which we shall later refer to as an \( \mathcal{A} \)-Hamiltonian vector field. In Euclidean space, we can show that (3) boils down to (1), thus showing that the integrability condition is not inherent to measure-preserving diffusions, but rather comes from the Fourier analysis used by the authors to derive the Euclidean recipe.

To derive this result, we begin in [4] by building on ideas from Poisson mechanics to construct a general \( P \)-preserving diffusion on \( M \) that naturally extends the Euclidean recipe (1). However, since the resulting diffusion is constructed from the Euclidean recipe, it does not take into account the non-trivial topological features of the sample space, and is thus incomplete, meaning that not every \( P \)-preserving
diffusion can be expressed in that form. To remedy this, we rely on the geometry induced by $P$ in §3 to derive the complete system (2). In §4 we discuss the important case when $M$ is compact, and show how the topological obstructions can be directly expressed using harmonic forms of an arbitrary Riemannian metric. The reversibility properties of (2) will then be discussed in §5, where we derive a general condition for the generator to be reversible up to some measure-preserving diffeomorphism, that generalises the momentum flip used in HMC to obtain a well-defined Metropolis–Hastings correction. In §6 we give an example of some new insights gained by the geometric formulation, by deriving a new recipe of volume-free $e^{-H} \mu_M$-preserving diffusions, a subclass of (3) in which the volume terms $\text{curl}_{\mu_M}(A)$ and $\text{div}_{\mu_M}(Y_i)Y_i$ vanish. The volume-free property is shared by both the underdamped and standard overdamped Langevin processes, and it not only simplifies the practical implementation of the diffusion, but confers it important geometric guarantees, making this volume-free subclass of diffusions particularly suited as a starting point to construct Langevin-like samplers. For the remaining sections, in §7 we study non-degenerate processes on manifolds, and characterise $P$-preserving diffusions that are expressed in terms of Riemannian Itô noise. In §8 we discuss the deterministic flow on the space of smooth measures associated to $P$-preserving diffusions, and derive a simple formula for the rate of change of functionals over measures, such as the KL divergence and other information entropies. In §9 we discuss the geometry and generalisation of the underdamped Langevin diffusions to manifolds, which we can use to construct an irreversible Langevin-based sampler, that generalises both the second-order Langevin HMC on $\mathbb{R}^n$, as well as the Euler–Poincaré diffusions on Lie groups, of which the original HMC algorithm is a special case. Finally, in §10 and §11 we briefly discuss the ergodicity and history of measure-preserving diffusions.

**Notation.** Throughout, $M$ is an arbitrary $n$-dimensional smooth manifold, and in particular, no assumptions are made on its connectedness, orientability, or compactness. We denote by $\mathfrak{X}^k(M)$ and $\Omega^k(M)$ the spaces of $k$-vector fields and $k$-forms, i.e., antisymmetric, contravariant and covariant tensor fields of rank $k$ respectively. The space of vector fields is denoted $\mathfrak{X}(M) \equiv \mathfrak{X}^1(M)$, and given $X \in \mathfrak{X}(M)$, $L_X$ denotes the associated Lie derivative. The exterior derivative on differential forms is denoted using the bold font $d$, and the space of smooth $\mathbb{R}$-valued functions on $M$ is denoted $C^\infty(M)$. We say that $P$ is a smooth measure if it is Radon measure that is absolutely continuous with respect to the null sets of the manifolds (generated by the charts). This means that over any coordinate chart $(x^i)$, we can write $P = p \, dx$, where $dx$ is the local Lebesgue measure, and $p : M \to \mathbb{R}$ is a measurable function, which we will assume to be smooth. We say that $P$ is positive if it is globally supported (its support is $M$) and its local densities $p$ above are positive smooth functions - in which case we denote its divergence on vector fields by $\text{div}_P : \mathfrak{X}(M) \to C^\infty(M)$, defined as $\text{div}_P(X)P = L_XP$, and let $L^2(P)$ be the space of square $P$-integrable $\mathbb{R}$-valued functions on $M$. Given a diffeomorphism $\mathcal{R} : M \to M$, we denote by $\mathcal{R}^*$ and $\mathcal{R}_*$ the induced pullback and pushforward on tensor fields respectively.

**Stochastic Differential Equations On Manifolds.** The standard Itô stochastic processes, such as the Wiener and Ornstein–Uhlenbeck processes, are typically defined over the real line. Multivariate stochastic processes over the real numbers
are then built up by injecting these processes along each coordinate axis. A general manifold, however, is not rigid enough to admit this kind of construction without being endowed with a connection, which allows a multivariate stochastic process to be defined locally and then developed into a stochastic process that evolves over the manifold [149, 125, 58, 136, 101]. Conveniently, Stratonovich processes do not require this machinery and can be defined over general manifolds using vector fields that direct the local noise [90, 101]. We shall denote the Stratonovich differential by $\circ d$, and the standard Brownian motion on $\mathbb{R}^N$ by $W_t$ [25, 140].

### 2. A General Measure-Preserving Diffusion on Manifolds

In this section, we present a step-by-step construction of a general class of measure-preserving diffusions that extends the Euclidean recipe (1) to manifolds in a natural way. To do this, our strategy is to inspect each term in (1) and replace them with its natural counterparts on manifolds, and finally showing that the resulting diffusion is indeed measure-preserving.

First, we replace the Lebesgue measure $dx$ on $\mathbb{R}^n$ with an arbitrary smooth and positive reference measure $\mu_M$ on $M$, hereafter referred to as the volume measure (note that there is no analogue of $dx$ on general non-homogeneous manifolds). Typically, $\mu_M$ is a measure that is canonically induced by additional structures on $M$, for instance a Haar, uniform, Riemannian or symplectic measure. The assumptions on the target $P$ guarantee that it can be written as a Gibbs distribution with respect to some “Hamiltonian” function $H : M \rightarrow \mathbb{R}$ and “inverse temperature” $\beta > 0$, given as

$$P \equiv p_\infty d\mu_M \propto e^{-\beta H} \mu_M.$$  

(4)

The Hamiltonian then represents the unnormalised log-density $H \propto \log p_\infty$ of the target measure.

Let us first consider the scenario in which the antisymmetric component $Q$ in (1) vanishes. In this case, we observe that the complete recipe consists of a general noise contribution $\sqrt{2D} dW_t$ associated to an arbitrary positive semi-definite matrix $D$, corrected by a drift component $(-D \nabla H + \nabla \cdot D) dt$. This latter drift term is obtained by the following well-known result [140, Prop. 4.5] (the notion of reversibility will be discussed carefully in §5).

**Proposition 2.1** ([134]). Given a vector field $X$ on $M = \mathbb{R}^n$, the target measure $P \equiv p_\infty dx$ is a solution to the stationary Fokker–Planck equation for the Itô SDE $dZ_t = X(Z_t) dt + \sqrt{2D} dW_t$ when

$$\nabla \cdot \mathcal{J}(p_\infty) = 0, \quad \text{where} \quad \mathcal{J}(p_\infty) \equiv p_\infty X - \nabla \cdot (p_\infty D).$$

Moreover, $dZ_t$ is a $p_\infty dx$-preserving reversible process, that is, the Fokker–Planck current $\mathcal{J}(p_\infty)$ vanishes, if and only if

$$dZ_t = \frac{1}{p_\infty} \nabla \cdot (p_\infty D) dt + \sqrt{2D} dW_t = (-D \nabla H + \nabla \cdot D) dt + \sqrt{2D} dW_t.$$ 

Hence, given the random noise $\sqrt{2D} dW_t$, the deterministic drift $(-D \nabla H + \nabla \cdot D) dt$ provides the necessary and sufficient correction to ensure that the diffusion is reversible with respect to the target measure $p_\infty dx$. To extend this idea to manifolds, we begin by replacing the Itô differential in the noise contribution $\sqrt{2D} dW_t$, with Stratonovich differentials, as these do not require a connection on $M$ [136].
Sec. 4]. Specifically, we replace the Itô noise $\sqrt{2d}dW_t$ with the Stratonovich noise $Y_t \circ dW_t^i$, where $\{Y_1, \ldots, Y_N\}$ is a generic family of ‘noise’ vector fields. To proceed further, we shall rely on the following useful result (proved in Appendix A.1).

**Lemma 2.2.** Given smooth vector fields $X, Y_1, \ldots, Y_N$ on $M$, consider the Stratonovich SDE

$$dZ_t = X(Z_t) \, dt + Y_t(Z_t) \circ dW_t^i.$$  

Its generator is given by $L f = X f + \frac{1}{2} Y_i(f) Y_i + \frac{1}{2} \text{div}_{\mu_M}(Y_i) Y_i$.

The Fokker–Planck operator, viewed as the formal adjoint of $L$ in $L^2(\mu_M)$ is then

$$L^* f = \text{div}_{\mu_M} \left( -f X + \frac{1}{2} Y_i(f) Y_i + \frac{1}{2} \text{div}_{\mu_M}(Y_i) Y_i \right).$$

Now, for $P$ to be an invariant measure of the system, it suffices to show that $L e^{-\beta H} = 0$. Mirroring the Euclidean case, we choose the drift $X$ to ensure that the Fokker–Planck current

$$\mathcal{Z}(f) \equiv -f X + \frac{1}{2} Y_i(f) Y_i + \frac{1}{2} \text{div}_{\mu_M}(Y_i) Y_i$$

vanishes when $f$ is the target density $e^{-\beta H}$. This leads to the choice

$$X \equiv -\frac{\beta}{2} Y_i(H) Y_i + \frac{1}{2} \text{div}_{\mu_M}(Y_i) Y_i,$$

which naturally replaces the term $-D \nabla H + \nabla \cdot D$ in the Euclidean recipe. Specifically, we have

$$\mathcal{Z}(e^{-\beta H}) = 0 \iff dZ_t = \left( -\frac{\beta}{2} Y_i(H) Y_i + \frac{1}{2} \text{div}_{\mu_M}(Y_i) Y_i \right) dt + Y_t \circ dW_t^i,$$

and in particular, the stationary Fokker–Planck equation

$$L^*(e^{-\beta H}) = \text{div}_{\mu_M}(\mathcal{Z}(e^{-\beta H})) = 0$$

is satisfied. We note that this is an instance of the fluctuation-dissipation relation, where the volume-distortion caused by the noise $Y_t \circ dW_t^i$ is exactly balanced by the volume-dissipative drift $X \equiv -\frac{\beta}{2} Y_i(H) Y_i dt + \frac{1}{2} \text{div}_{\mu_M}(Y_i) Y_i$.

We now consider the general case in which $Q$ does not necessarily vanish. We note that geometrically, the drift term $Q \nabla H$ in (1) represents a vector field that depends linearly on the gradient of the log-density $H$. While manifolds are generally nonlinear spaces, their tangent and cotangent bundle provide linear spaces over each point $x \in M$, namely, the tangent space $T_x M$ of vectors, to which $Q \nabla H|_x$ belongs, and the cotangent space $T^*_x M$ of covectors, to which $\nabla H|_x$ belongs.

Geometrically, maps from $\Omega^1(M)$ to $\mathfrak{X}(M)$, such as $\nabla H \mapsto Q \nabla H$ that are linear at each point on $M$ are called vector bundle morphisms, since they are compatible with the vector bundle structures. A vector bundle morphism can be conveniently represented using a bracket $\mathcal{B} \in \Gamma(TM \otimes TM)$ (i.e., a contravariant tensor field of rank two), which assigns to the log-density $H$, a $\mathcal{B}$-Hamiltonian vector field $X^\mathcal{B}_H$ via the relation $X^\mathcal{B}_H \equiv \mathcal{B}(dH, \cdot)$. Hence, we deduce that the linear operator $Q$ may be interpreted as a bracket $\mathcal{B}$ on manifolds and the vector field $X^\mathcal{B}_H$ is a natural candidate for generalising the term $Q \nabla H$ in the Euclidean recipe.

**Example 2.3.** $\mathcal{B}$-Hamiltonian vector fields are ubiquitous in science. For example, they include Riemannian gradient flows, Hamiltonian vector fields associated to Poisson structures, and in particular the ones associated to a symplectic structure, 4-gradient vector fields generated by a Lorentzian metric over spacetime, and thermodynamic flows, which we shall come back to in §5.
On the other hand, it is not a-priori clear how to interpret the final term “∇ · $Q$” in (1) intrinsically, as this would mean “differentiate the rank two tensor field $B$ to turn it into a vector field” – such an operation does not exist on general manifolds.

To proceed, we make the following ansatz for the measure-preserving diffusion on $M$

$$(7) \quad dZ_t = (X^B_H + Y)dt + ( - \frac{1}{2} \beta Y_i(H)Y_i + \frac{1}{2} \text{div}_{\mu_M}(Y_i)Y_i)dt + Y_i \circ dW_i^t,$$

where $Y$ is currently an unspecified vector field that will later generalise the term “$\nabla \cdot Q$” in (1). Meanwhile, we have the following result (proof in §A.2):

**Theorem 2.4.** The Gibbs measure (1) is preserved under the bracket diffusion (7) if and only if the vector field $Y$ satisfies

$$(8) \quad \text{div}_{\mu_M}(X^B_{p_{\infty}} - \beta p_{\infty} Y) = 0.$$  

We shall now use this result to make sense of the vector field $Y$. Observe that by analogy with the Euclidean case, we want to obtain a complete recipe that is valid for any target distribution $P$, and thus for any choice of density $p_{\infty}$ with respect to a convenient volume measure $\mu_M$. Since $Y$ should not depend on the choice of the target density, we expect the identity (8) to hold for any positive density $p_{\infty}$. In particular, setting $p_{\infty} \equiv$ constant, we have $X^B_{p_{\infty}} = 0$, implying that $Y$ must preserve the reference measure, i.e., $\text{div}_{\mu_M}(Y) = 0$. If we assume this latter condition, then (8) can be written as

$$(9) \quad \text{div}_{\mu_M}(X^B_{p_{\infty}}) = \beta Y(p_{\infty}),$$

which holds for any density $p_{\infty}$. When $B$ is a Poisson structure (i.e., it is antisymmetric and satisfies the Jacobi identity), equation (9) is precisely the definition of modular vector fields $Y$ in Poisson mechanics (see [51, 52, 159]). Specifically, we can associate to a bracket $B$ and a volume measure $\mu_M$, a modular vector field $X^B_M$, which is defined as the differential operator

$$(10) \quad X^B_M : f \mapsto \text{div}_{\mu_M}(X^B_f),$$

acting on smooth functions. While we have no reason to require that $B$ is Poisson, it is necessary for it to be antisymmetric in order for $X^B_M$ to be a vector field, otherwise it will not satisfy the derivation property $X^B_M(fg) = fX^B_M(g) + gX^B_M(f)$.

Hereafter, we shall denote an arbitrary antisymmetric bracket by $A \in \mathfrak{X}(M)$, and note that the associated $A$-Hamiltonian vector field $X^A_H$ preserves the target density, i.e. $\mathcal{L}_{X^A_H} p_{\infty} = 0$, so the integral curves of $X^A_H$ remain tangent to the surfaces of constant target density. Thus, replacing $Y$ with $X^M_A$ in (7), we obtain the following class of diffusions

$$(11) \quad dZ_t = \underbrace{X^B_H dt}_{\mu_M \text{-preserving}} + \underbrace{\beta^{-1} X^B_M dt}_{\mu_M \text{-preserving}} - \underbrace{\frac{1}{2} \beta Y_i(H)Y_i dt}_{\mu_M \text{-preserving}} + \underbrace{\frac{1}{2} \text{div}_{\mu_M}(Y_i)Y_i dt}_{\mu_M \text{-preserving}} + \underbrace{Y_i \circ dW_i^t}_{\mu_M \text{-preserving}},$$

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1To see this, check that $X^M_A(fg) = \text{div}_{\mu_M}(fX^M_A + gX^M_f) = B(dg, df) + fX^M_A(g) + B(df, dg) + gX^M_A(f)$
which, by construction, preserves the target measure $P \propto e^{-\beta H} \mu_M$. Moreover, in the Euclidean case, (11) recovers the Euclidean diffusion

$$dZ_t = -Q \nabla H dt + \nabla \cdot Q dt - D \nabla H dt + \nabla \cdot D dt + \sqrt{2D} dW_t,$$

as shown in the following result (see proof in §A.3).

**Corollary 2.5.** Let $M = \mathbb{R}^n$, $\mu_M = dx$, $\sigma_{ij} \equiv Y^i_j$, $D \equiv \frac{1}{2} \sigma \sigma^T$ and $Q_{ij} \equiv A^{ij}$. Then (11) reduces to the Itô diffusion (1) derived in [121].

**Remark 2.6.** We warn the readers about the similarity in the notations used for $\mathcal{A}$-Hamiltonian vector fields $X^P_{\mathcal{A}}$ and modular vector fields $X^\mu_{\mathcal{A}^\mu}$. In the former, the bi-vector field $\mathcal{A}$ appears in the superscript, with a scalar function appearing in the subscript, while in the latter, the bi-vector field $\mathcal{A}$ appears in the subscript, with a positive measure appearing in the superscript.

So far, we have explained how to give intrinsic meaning to each term of (1) and constructed a class of diffusions that preserve the measure $P$. However, it is still unclear at this point whether this class of diffusions (11), hereafter referred to as $\mathcal{A}$-diffusions, is complete, that is, whether any $P$-preserving diffusion on $M$ has the form (11). In the following, we shall answer this question by taking into account the geometry of volume manifolds, given by the tuple $(M, P)$, where $P$ is a smooth positive measure on $M$.

### 3. Local and Global Completeness of $\mathcal{A}$-Diffusions

To work with the geometry and topology of $M$ induced by our smooth positive target measure $P$, we rely on the $P$-musical isomorphisms, defined as follows. Let $\Omega^k_{\text{Or}}(M)$ be the space of $k$-twisted differential forms introduced by de Rham [46] (see for example [63], Sec. 2.8) for an introduction to these important objects, while the unfamiliar reader may treat them as standard differential $k$-forms with loss of generality. The $P$-flattening operator $P^\flat : \mathfrak{X}^k(M) \to \Omega^n_{\text{Or}}(M)$ for integers $0 \leq k \leq n$ is defined by $P^\flat(X) \equiv i_X P$, where $i_X$ denotes the interior product of (twisted) differential forms with a $k$-vector field $X$ [38][127]. More precisely, $P^\flat(X)$ is a twisted $(n-k)$-differential form such that for any $(n-k)$-vector field $W$, we have

$$P^\flat(X)(W) = \langle P^\flat(X), W \rangle_* \equiv \langle i_X P, W \rangle_* = \langle P, i_X W \rangle_*,$$

where $\langle \cdot, \cdot \rangle_* : \Omega^k(M) \times \mathfrak{X}^k(M) \to C^\infty(M)$ denotes the duality pairing. Note that this map is well-defined regardless of whether $P$ is positive or not. When $P$ is globally supported, it becomes a $C^\infty(M)$-linear isomorphism

$$P^\flat : \mathfrak{X}^k(M) \isom \Omega^n_{\text{Or}}(M),$$

with the inverse denoted by $P^\sharp$. We refer to the maps $P^\flat$ and $P^\sharp$ as the $P$-musical isomorphisms, which should not be confused with the Riemannian musical isomorphisms.

**Example 3.1.** As an interesting example that shows the relevance of the $P$-musical isomorphisms in the context of statistics, observe that if $Q$ is a smooth measure on $M$, then $P^\sharp$ yields the Radon–Nikodym derivative

$$P^\sharp(Q) = \frac{dQ}{dP}.$$
which can be observed directly from \( Q = f P = P^b(f) \), where \( f = \frac{dQ}{dt} \in C^\infty(M) \).

Crucially for our purpose, the \( P \)-musical isomorphisms \( P^b \) and \( P^d \) allow us to construct a canonical derivative associated to \( P \), which will be central to our discussion on the completeness of \( \mathcal{A} \)-diffusions.

**Definition 3.2 ([27]).** The \( P \)-rotationnel of a \( k \)-vector field for some integer \( 1 \leq k \leq n \) is defined as

\[
\text{curl}_P \equiv P^d \circ \text{d} \circ P^b : \chi^k(M) \to \chi^{k-1}(M),
\]

where \( \text{d} \) also denotes the extension of the exterior derivative to twisted forms [27]. When \( k = 0 \), we set \( \text{curl}_P(f) \equiv 0 \) for any \( f \in C^\infty(M) \).

An important property of the operator \( \text{curl}_P \) is that it does not depend on the normalisation of \( P \) (i.e., if \( a \in \mathbb{R} - \{0\} \), then \( \text{curl}_{aP} = \text{curl}_P \)), which is often unknown in applications. This is the case for example in Bayesian statistics (the posterior distribution), and in molecular dynamics (the canonical distribution).

In the context of measure-preserving diffusions, we are particularly interested in the action of \( \text{curl}_P \) on vector fields and bi-vector fields, which is given as follows.

In the case \( k = 1 \) (i.e., vector fields), the \( P \)-rotationnel recovers the divergence operator

\[
\text{curl}_P|_{\chi(M)} = \text{div}_P,
\]

and in the case \( k = 2 \) (i.e., bi-vector fields), we have the following result showing that \( \text{curl}_P \) maps bi-vector fields to their modular vector field [10] (proved in §A.4).

**Theorem 3.3.** Given a volume manifold \((M, P)\), we have the identity

\[
\text{curl}_P(\mathcal{A}) = X^P_A.
\]

It follows that we can replace the terms \( X^P_M \) and \( \text{div}_{\mu_M}(Y_i)Y_i \) in (11) by \( \text{curl}_{\mu_M}(\mathcal{A}) \) and \( \text{curl}_{\mu_M}(Y_i)Y_i \) respectively, suggesting that the rotationnel plays a central role in the construction of measure-preserving diffusions. To realise the full potential of \( \text{curl}_P \) in our context, we need the following lemma (proved in §A.5).

**Lemma 3.4.** The Fokker–Planck operator of the SDE (10), viewed as the formal adjoint of the generator \( \mathcal{L} \) with respect to the dual pairing \( \langle f, P \rangle_c \mapsto \int f dP \) between smooth compactly supported functions \( f \) and smooth measures \( P \), is given by

\[
\mathcal{L}^*P = -\mathcal{L}_X P + \frac{1}{2} \mathcal{L}_{Y_i} \mathcal{L}_{Y_i} P.
\]

If \( P \) is also positive, then the density of the smooth measure \( \mathcal{L}^*P \) with respect to \( P \) is given by \( \text{div}_P \left( \frac{1}{2} \text{div}(Y_i)Y_i - X \right) \), and we call

\[
\mathcal{J}(P) \equiv \frac{1}{2} \text{div}(Y_i)Y_i - X
\]

the **Fokker-Planck current** of \( P \). Thus

\[
\mathcal{L}^* P = \text{curl}_P(\mathcal{J}(P))P = \text{div}_P(\mathcal{J}(P))P.
\]

Hence, the condition that \( P \) is preserved by the diffusion, namely \( \mathcal{L}^* P = 0 \), reduces to the condition that its Fokker–Planck current is \( P \)-preserving, i.e.,

\[
\mathcal{L}^* P = 0 \iff \text{div}_P(\mathcal{J}(P)) = 0.
\]

Now, as discussed in §B the \( \mathbb{R} \)-linearity of \( \text{curl}_P \), combined with the fact that it satisfies

\[
\text{curl}_P \circ \text{curl}_P = P^d \circ \text{d} \circ P^b \circ P^d \circ \text{d} \circ P^b = P^d \circ \text{d} \circ \text{d} \circ P^b = 0,
\]
where we used that \( \mathbf{d} \circ \mathbf{d} = 0 \), implies that \( \text{curl}_P \) is a boundary operator on the space of multi-vector fields. Accordingly, the measure \( P \) defines homology groups

\[
\mathcal{H}_P^k(M) \equiv \frac{\ker(\text{curl}_P : \mathfrak{X}^k(M) \to \mathfrak{X}^{k-1}(M))}{\text{Im}(\text{curl}_P : \mathfrak{X}^{k+1}(M) \to \mathfrak{X}^k(M))}
\]

that inform us about the properties of \( \text{curl}_P \)-free multi-vector fields on \( (M, P) \). In particular, the first homology group \( \mathcal{H}_P^1(M) \) of \( P \) describes the discrepancy between \( \text{div}_P \)-free vector fields and curl vector fields, i.e., vector fields of the form \( \text{curl}_P(A) \) for some \( A \in \mathfrak{X}^2(M) \), and it follows that the space of \( \text{div}_P \)-free vector fields, to which the Fokker–Planck current \( \mathfrak{J}(P) \) of \( P \)-preserving diffusions belongs, is isomorphic to

\[
\ker(\text{div}_P : \mathfrak{X}(M) \to C^\infty(M)) \cong \text{Im}(\text{curl}_P : \mathfrak{X}^2(M) \to \mathfrak{X}(M)) \oplus \mathcal{H}_P^1(M).
\]

As a result, any \( P \)-preserving vector field \( Z \in \mathfrak{X}(M) \), i.e., \( \text{div}_P(Z) = 0 \), can be expressed as a sum of (1) a globally curled component \( \text{curl}_P(A) \) for some \( A \in \mathfrak{X}^2(M) \), and (2) an additional term belonging to the first homology group \( \mathcal{H}_P^1(M) \), associated to topological obstructions.

It remains to characterise the elements of these groups, which can be achieved by noting that the \( P \)-musical isomorphism \( P^d \) induces isomorphisms between the homology groups \( \mathcal{H}_P^k(M) \) and the twisted de Rham cohomology groups \( \mathcal{H}^{n-k}_{dR}(M) \) (see remark 3.5), implying that

\[
\mathcal{H}_P^1(M) \cong P^d(\mathcal{H}^{n-1}_{dR}(M)).
\]

Thus, the additional topological obstruction term may be parametrised by \( P^d(\gamma) \), where \( \gamma \) is a closed, twisted \( (n-1) \)-form whose de Rham class is non-zero. In conclusion, any such \( Z \) can be expressed as

\[
Z = \text{curl}_P(A) + P^d(\gamma),
\]

with \( A \in \mathfrak{X}^2(M) \) and \( \gamma \in \mathcal{H}^{n-1}_{dR}(M) \) (see theorem 3.4 for more details).

**Remark 3.5 (Twisted de Rham Cohomology).** The twisted de Rham cohomology groups, defined as [27]

\[
\mathcal{H}^k_{dR}(M) \equiv \frac{\ker(\mathbf{d} : \Omega^k_{\text{Or}}(M) \to \Omega^{k+1}_{\text{Or}}(M))}{\text{Im}(\mathbf{d} : \Omega^k_{\text{Or}}(M) \to \Omega^k_{\text{Or}}(M))},
\]

describe the topology of the sample manifold \( M \), such as the number of connected components of an orientable manifold \( M \), which is given by the 0-th twisted de Rham cohomology group \( \mathcal{H}^0_{dR}(M) \). They also provide information on the solutions to the equation \( d\alpha = \beta \) [103] Chap. 18. Similarly, the measure-informed homology groups \( \mathcal{H}^{n-k}_{dR}(M) = P^d(\mathcal{H}^k_{dR}(M)) \) inform us about the solutions of the equation \( \text{curl}_P(V) = \mathcal{W} \), of which the stationary Fokker–Planck equation [14] is a special case.

**Remark 3.6 (Fokker–Planck Operators).** The Fokker–Planck operator was defined as the adjoint of \( \mathcal{L} \) with respect to the pairing \( \langle f, P \rangle_* = \int_M f \mathbf{d}P \). However in the previous section, it was defined as the adjoint with respect to the pairing \( C^\infty_c(M) \times C^\infty_c(M) \to \mathbb{R} \) defined as \( \langle f, h \rangle_{\mu_M} = \int f h \mathbf{d}\mu_M \). The difference between these two pairings is that the former is a special case of the standard Poincaré bilinear form on the manifold \( M \), i.e., \( \langle \alpha, \beta \rangle_* = \int \alpha \wedge \beta \), while the latter is associated to the induced measure-informed bilinear form via the \( P \)-musical flattening, that
The relation between the various definitions of the Fokker–Planck operator is then
\[ \langle \mathcal{L} f, P \rangle_* = \langle f, \mathcal{L}^* P \rangle_* = \langle f, \text{div} P(\mathfrak{H}(P)) \rangle_* = \langle f, \text{div} P(\mathfrak{H}(e^{-H})) \rangle_{\mu M}. \]

When focussing on just the local representations of $P$-preserving diffusions, we can also use the musical isomorphisms of $P$ to consider a “$P$-twisted” Poincaré lemma\(^2\), which states that any vector field $Z$ that preserves the measure $P$ can be expressed locally as curled vector fields (see theorem B.1). More precisely, this means that we can find a neighbourhood $\iota_U : U \to M$ around any point in $M$, where $\iota_U$ is the inclusion, and a locally defined $\mathcal{A} \in \mathfrak{X}^2(U)$ for which
\[ Z|_U = \text{curl}_{\iota_U}^* P(\mathcal{A}) \]
holds. Combining these results with the fact that the Fokker–Planck current of $P$-preserving diffusions is $\text{div} P$-free, we obtain the following complete characterisation, or recipe, of $P$-preserving diffusions:

**Theorem 3.7** (Local and global completeness of $\mathcal{A}$-diffusions). The smooth, positive target measure $P$ is a stationary measure of the general diffusion process
\[ dZ_t = X(Z_t)dt + Y_t(Z_t) \circ dW^i_t \]
if and only if the drift takes the form $X = \text{curl}_{\iota_U}^* P(\mathcal{A}) + \frac{1}{2} \text{div}_{\iota_U}^* P(Y_t)Y_t$ on a neighbourhood $\iota_U : U \to M$ of any point, for some local antisymmetric bracket $\mathcal{A} \in \mathfrak{X}^2(U)$. Thus, any such diffusions may be locally represented as
\[ dZ_t = \text{curl}_{\iota_U}^* P(\mathcal{A})dt + \frac{1}{2} \text{div}_{\iota_U}^* P(Y_t)Y_t dt + Y_t(Z_t) \circ dW^i_t, \]
which we will also refer to as $\mathcal{A}$-diffusions since as discussed below, they recover the original $\mathcal{A}$-diffusions \[11\] when $P$ is written in the form \[4\]. Hence, the class of $\mathcal{A}$-diffusions is locally complete. Furthermore, they are globally complete, that is, any $P$-preserving diffusions is of the form \[16\] globally, if and only if the first homology group of $P$, or equivalently the $(n-1)^{st}$ twisted de Rham cohomology group, is trivial. More generally, any $P$-preserving diffusion on any manifold can be expressed as
\[ dZ_t = \left( \text{curl}_P(\mathcal{A}) + P^2(\gamma) + \frac{1}{2} \text{div}_P(Y_t)Y_t \right) dt + Y_t(Z_t) \circ dW^i_t, \]
for some $\mathcal{A} \in \mathfrak{X}^2(M)$, and $\gamma \in H^{n-1}_{dR}(M)$.

We stress that this result not only generalises the complete recipe derived in \[121\], but also provides a re-interpretation of its derivation in terms of the canonical geometry of the target measure $P$. A parallel can be made with the construction of potentials in physics. Indeed, conservative fields in physics are usually represented by potentials. For example in classical mechanics, the Newton force $F$ is conservative if the net work done by it along any two (piecewise smooth) paths $\lambda, \lambda$ with the same end points is the same, i.e., $\int_\lambda F = \int_\lambda F$. \[103\] theorem 11.42. Such force fields are represented by potential energy functions $V$, so we can find $V$ such that $F = dV$. Similarly, in the theory of electromagnetism, Gauss’s and Faraday’s laws may be represented in the form $d\mathbf{F} = 0$, where $\mathbf{F}$ is the electromagnetic 2-form.

---

\(^2\)The standard Poincaré lemma states that any closed differential form $\alpha$ can be expressed locally as an exact form $d\beta$. The ‘$P$-twisted’ Poincaré lemma is the measure-informed analogue to this on the space of multi-vector fields.
These laws are equivalent to the existence of a magnetic potential $1$-form $A$ for which $F = dA$ \[3\].

The situation is analogous in the context of $P$-preserving diffusions, except that we need to adjust to the geometry induced by the target $P$, and use its canonical differential operator $\text{curl}_P$ in place of the exterior derivative $d$. As mentioned above, the condition that the diffusion \[14\] preserves $P$ is simply a condition that the Fokker–Planck current $\mathcal{J}(P) = \int_x \text{div}_P(Y_i)Y_i - X$ conserves $P$, i.e., $\text{div}_P(\mathcal{J}(P)) = 0$. Such conservative currents are locally represented by a ‘potential’ $A$, i.e., $\mathcal{J}(P) = \text{curl}_P(A)$. Surprisingly, this procedure is entirely canonical: it only depends on the volume manifold $(M, P)$, which are the only objects we are given a-priori in many applications. In particular on $M = \mathbb{R}^n$, the de twisted de Rham cohomology is trivial, so this procedure holds globally. Thus we recover the result that if $Z$ is divergence-free (with respect to the Lebesgue measure), i.e., $\nabla \cdot Z = 0$, then there exists an antisymmetric matrix $A$ for which $Z = \nabla \cdot A$ \[30\]. This is all that is needed to obtain the Euclidean complete recipe of \[21\]. Consequently, our result shows that the integrability assumption in \[121\] is not needed – it is precisely the expression for curl $\mu$-preserving vector field $\text{curl}_P$ has a natural gauge freedom obtained by adding a constant to $V$, $V \mapsto V + c$ (which is the reason why HMC does not require knowledge of the normalising constant of the target measure).

Finally, to recover the $A$-diffusion \[11\] expressed in terms of a reference measure $\mu_M$ from the canonical $A$-diffusion \[10\], we simply need to express the curl of $P = e^{-H} \mu_M$ in terms of the curl of $\mu_M$, which may be achieved by noting that

$$\text{curl}_P(A) = \frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y} = \mu_M^y \circ dH \circ \mu_M^x,$$

where $dH \equiv d - dh \wedge \cdot$ is the ‘distorted’ exterior derivative \[73\] \[148\]. This is precisely the expression for $\text{curl}_{\mu_M}$ with $d$ replaced by $dH$ and one can check that the additional ‘twist’ $dH \wedge \cdot$ generates both log-density terms $X^3_H$ and $Y_i(H)Y_i$ in \[11\] (see \[3.6\] for a more detailed derivation). Hence, if $P = e^{-H} \mu_M$, we have

$$\text{curl}_P(A) = \text{curl}_{\mu_M}(A) + X^A_H = X^\mu_M + X^A_H, \quad \text{div}_P(Y_i)Y_i = \text{div}_{\mu_M}(Y_i)Y_i - Y_i(H)Y_i.$$

It is interesting to observe that the $P$-preserving vector field $\text{curl}_P(A)$ always splits into a volume-preserving term $X^A_H$, i.e., $\mathcal{L}_{X^A_H} \mu_M = 0$, and a density-preserving term $X^\mu_M$, i.e., $\mathcal{L}_{X^\mu_M} \mu_M = 0$.

Remark 3.8. Let us briefly explain why $\text{curl}_{\mu_M}$ is called ‘curl’. Note that when $M = \mathbb{R}^3$ and $\mu_M = dx \equiv dx \, dy \, dz$, we can write any bi-vector field $A \in \mathfrak{X}^2(\mathbb{R}^3)$ as $A = A_x \partial_x \wedge \partial_x + A_y \partial_y \wedge \partial_x + A_z \partial_z \wedge \partial_y$, and $\text{curl}_{\mu_M}$ corresponds to the classical curl of the “vector field” $(A_x, A_y, A_z)$:

$$\text{curl}_{\mu_M}(A) = \left( \frac{\partial A_y}{\partial z} - \frac{\partial A_z}{\partial y} \right) \partial_x + \left( \frac{\partial A_z}{\partial x} - \frac{\partial A_x}{\partial z} \right) \partial_y + \left( \frac{\partial A_x}{\partial y} - \frac{\partial A_y}{\partial x} \right) \partial_z.$$
In particular, any $d\mathbf{x}$-preserving vector field can be written as above, which we may also view as a sum of Hamiltonian vector fields on the coordinate 2-surfaces:

\[
\text{curl}_{d\mathbf{x}}(\mathbf{A}) = \left( \frac{\partial A_y}{\partial z} \frac{\partial x}{\partial} - \frac{\partial A_y}{\partial x} \frac{\partial z}{\partial} \right) + \left( \frac{\partial A_z}{\partial y} \frac{\partial y}{\partial} - \frac{\partial A_z}{\partial y} \frac{\partial y}{\partial} \right) + \left( \frac{\partial A_x}{\partial z} \frac{\partial z}{\partial} - \frac{\partial A_x}{\partial z} \frac{\partial x}{\partial} \right).
\]

(Recall the Hamiltonian vector field of $H$ in Darboux coordinates $(q, p)$ is $\frac{\partial H}{\partial p} \frac{\partial}{\partial q} - \frac{\partial H}{\partial q} \frac{\partial}{\partial p}$.)

Remark 3.9. In the Euclidean space recipe, the terms associated with the $2^{nd}$-order tensors $\nabla \cdot D$ and $\nabla \cdot Q$ look identical – they are obtained by applying the “divergence” $\nabla \cdot$ to $D$ and $Q$, which are both second-order objects (i.e., tensors with two indices). In our geometric formulation, we observe that $\nabla \cdot D$ is actually obtained by differentiating the noise vector fields $\text{div}_P(Y_i)Y_i$ which are first-order tensors, while $\nabla \cdot Q$, corresponding to the term $\text{curl}_P(\mathbf{A})$ in our formulation, genuinely involves differentiating a second-order tensor $\mathbf{A}$. In particular, while it is true that $\text{curl} \circ \text{curl} = 0$, the equality $\nabla \cdot \nabla \cdot = 0$ is only valid when applied to the antisymmetric component, i.e.,

$\nabla \cdot \nabla \cdot D \neq 0, \quad \nabla \cdot \nabla \cdot Q = 0.$

The geometric formulation properly distinguishes these operations:

$\text{div}_{\mu \lambda M} (\text{div}_{\mu \lambda M} (Y_i)Y_i) = Y_i (\text{div}_{\mu \lambda M} (Y_i)) + (\text{div}_{\mu \lambda M} (Y_i))^2, \quad \text{div}_{\mu \lambda M} (\text{curl}_{\mu \lambda M} (\mathbf{A})) = 0,$

so that while $\text{curl}_{\mu \lambda M} (\mathbf{A})$ is always volume-preserving, this is generally not the case for $\text{div}_{\mu \lambda M} (Y_i)Y_i$ (an important exception is the Langevin diffusion as we shall discuss in §6).

In the next section we will describe the important scenario where the sample space $\mathcal{M}$ is compact, in which case the topological obstructions can be represented explicitly in terms of harmonic forms.

4. MEASURE-PRESERVING DIFFUSIONS ON COMPACT MANIFOLDS

We saw previously that when the topology of the sample space contain topological obstructions, it is necessary to add an additional term in $\mathcal{A}$-diffusions representing the non-triviality of the homology of $P$. For compact orientable manifolds, we may use the de Rham–Hodge–Kodaira’s decomposition of differential forms to construct the Fokker–Planck current of general $P$-preserving measures, as shown in the following theorem (proved in §A.7).

Theorem 4.1. Let $\mathcal{M}$ be a compact orientable Riemannian manifold and let $\mu_\mathcal{M} \equiv \text{vol}$ and $\nabla$ denote respectively the Riemannian measure and divergence. Then, any $e^{-H}$ vol-preserving diffusion has the form

\[
dZ_t \equiv (X_H + \frac{1}{2} (\nabla \cdot Y_i - Y_i(H)) Y_i - \nabla \cdot \mathbf{A} + e^H \ast \ast^{-1} \zeta) dt + Y_i \circ dW^i_t,
\]

where $\ast$ is the Hodge star operator, $\ast$ is the Riemannian musical isomorphism, $\mathbf{A}$ is an antisymmetric tensor and $\zeta$ is a harmonic $(n - 1)$-form (i.e., it satisfies “Maxwell’s equations” $d\zeta = 0, \ast d \ast \zeta = 0$).

A similar result can be found in [90], although the authors assume that the diffusion is also non-degenerate (i.e., its generator is elliptic) in order to obtain a Riemannian metric from the noise process (the Riemannian Brownian motion),
which is then used to turn the Fokker–Planck current \( J(P) \) into a 1-form that can be analysed through its de Rham–Hodge–Kodaira decomposition. In order to clarify the roles played by the assumptions of compactness and non-degeneracy, we have treated them separately, the latter which can be found in §7.

Note that in the above theorem 4.1, we do not make any assumptions on the noise, although it assumes that we can express our target measure \( P \) in terms of the Riemannian measure \( \text{vol} \), which might be inconvenient in practice. Topologically, the presence of the harmonic term in (17) may be understood from the fact that on compact orientable manifolds, the twisted de Rham cohomology groups are isomorphic to the space of harmonic forms. It follows that \( P \)-preserving vector fields have the form \( \text{curl}_P(\mathcal{A}) + P^1(\zeta) \) for an antisymmetric bracket \( \mathcal{A} \) and a non-zero harmonic \((n-1)\)-form \( \zeta \) (see §B). Hence, on compact manifolds, any \( P \)-preserving diffusions take the form

\[
\frac{dZ_t}{dt} = \underbrace{\text{curl}_P(\mathcal{A}) dt + \frac{1}{2} \text{div}_P(Y_t) Y_t dt + Y_t \circ dW_t}_\text{\(\mathcal{A}\)-diffusion} + \underbrace{P^2(\zeta) dt}_\text{harmonic obstruction},
\]

for some harmonic \((n-1)\)-form \( \zeta \) associated to an arbitrary Riemannian metric.

5. Reversibility

Recall that the Euclidean recipe for measure-preserving diffusions \( (1) \) depends entirely on an antisymmetric matrix \( Q \) and a symmetric positive semi-definite matrix \( D \). On the other hand, the geometric generalisation we have derived in previous sections is constructed using a bi-vector field \( \mathcal{A} \) and a set of noise-vector fields \( (Y_t) \). In order to make this connection clearer, we now discuss the symmetric/antisymmetric decomposition of \( \mathcal{A} \)-diffusions and its relation to the notion of reversibility. For this, we first note that the noise vector fields \( \{Y_i\}_{i=1}^N \) canonically generate a symmetric bracket, denoted \( S \equiv Y_i \otimes Y_i \), by setting

\[
S(\text{df}, \text{dg}) \equiv Y_i(f)Y_i(g) \quad \text{for any } f, g \in C^\infty(M).
\]

Introducing the notation

\[
\{f, g\}_B \equiv B(\text{df}, \text{dg}),
\]

for a general bracket \( B \), we see that the symmetric bracket defined above is dissipative, in the sense that it satisfies the dissipative property

\[
\{f, f\}_S = \sum_i Y_i(f)^2 \geq 0,
\]

which further implies

\[
\{f, g\}_S^2 \leq \{f, f\}_S \{g, g\}_S.
\]

This contrasts with the antisymmetric bracket, which has the conservative property

\[
\{f, f\}_{\mathcal{A}} = 0.
\]

Remark 5.1. In the context of mechanics, special forms of (symmetric) dissipative brackets \( S \) have been considered by several authors to model dissipative components of mechanical systems in an attempt to cast these systems from an algebraic framework. Examples include the metriplectic bracket [93, 132, 74, 76, 129], double-bracket [32, 26], and selective-decay bracket [67]. Whereas in these works the symmetric structures are constructed in an ad hoc manner, it would be interesting to understand them as arising from noise vector fields chosen to model fluctuations,
as we do here. This connection shall be further explored in a separate paper by the authors.

**Example 5.2.** When the bi-vector field $\mathcal{A}$ has nice properties such as symmetries, it can be desirable to employ it to construct the noise vector-fields. This may be done using “noise functions” $(H_i)$ and choosing $Y_i \equiv X_H^{\beta}$. Such a mechanism was used to construct a coordinate-independent irreversible MCMC sampler on Lie groups in [7]. In that case, the bracket $S$ satisfies $S(df, dg) = \mathcal{A}(dH_i, df)\mathcal{A}(dH_i, dg)$, and the generator of the diffusion has a double bracket form (this should not be confused with the notion of “double brackets” in the sense of Brockett and Bloch).

A bracket that is decomposed into the sum of an antisymmetric and dissipative bracket is known as a *thermodynamic bracket*. It follows that $P$-preserving diffusions are parametrised by thermodynamic brackets up to topological obstructions. Thus, many properties of the diffusion can be studied through its thermodynamic bracket; for example in [8] we will see that the thermodynamic bracket of the diffusion provides a simple formula to evaluate the rate of change of functionals on volume measures along the diffusion.

If we define the divergence of the dissipative bracket $S$ constructed above by $\text{div}_P(S) \equiv \text{div}_P(Y_i)Y_i$, we can decompose the drift of the $\mathcal{A}$-diffusion into components associated with the dissipative and antisymmetric brackets:

$$dZ_t = \underbrace{\text{curl}_P(\mathcal{A})}_\text{antisymmetric} dt + \underbrace{\frac{1}{2}\text{div}_P(S)}_\text{dissipative} dt + \underbrace{Y_i \circ dW^i}_\text{noise},$$

which for $P = e^{-\beta H}\mu_M$, further decomposes into (compare with (11))

$$dZ_t = \beta \left( X_H^\beta - \frac{1}{2}X^\delta_H \right) dt + \left( \frac{1}{2}\text{div}_{\mu_M}(S) + \text{curl}_{\mu_M}(\mathcal{A}) \right) dt + Y_i \circ dW^i.$$

The following corollary derives a decomposition of the corresponding generator into symmetric and anti-symmetric parts, generalizing the standard result in the Euclidean case [10]. This result is useful as for instance, it enables us to build the most general Stein operators on manifolds available from the generator approach.

**Corollary 5.3.** The generator of a $P$-preserving diffusion expressed in the form of (2) can be written as (recall the definition of the differential operator $X^P_\mathcal{A}$ in (10))

$$\mathcal{L}f = X^\mathcal{A}_P(f) + \underbrace{\mathcal{P}^\mathcal{A}(\gamma)(f)}_{\text{L}^2(P)-\text{symmetric}} + \underbrace{\frac{1}{2}X^\mathcal{P}_\mathcal{S}(f)}_{\text{L}^2(P)-\text{antisymmetric}}.$$

Moreover, $\frac{1}{2}X^\mathcal{P}_\mathcal{S}$ is symmetric in $L^2(P)$, while $X^\mathcal{A}_P$ and $\mathcal{P}^\mathcal{A}(\gamma)$ are both antisymmetric in $L^2(P)$. That is,

$$\langle X^\mathcal{A}_P f, h \rangle_P = -\langle f, X^\mathcal{A}_P h \rangle_P, \quad \langle X^\mathcal{P}_\mathcal{S} f, h \rangle_P = \langle f, X^\mathcal{P}_\mathcal{S} h \rangle_P,$$

where $\langle \cdot, \cdot \rangle_P$ denotes the $L^2(P)$ pseudo-inner product, $\langle f, h \rangle_P \equiv \int f h\,dP$. Hence, the generator $\mathcal{L}$ is symmetric if and only if $X^\mathcal{A}_P + \mathcal{P}^\mathcal{A}(\gamma) = 0$. In general, the generator of (10) satisfies $\mathcal{L} = \frac{1}{2}X^\mathcal{P}_\mathcal{S}$ if and only if the Fokker-Planck current of $P$ vanishes, in which case, we say that $\mathcal{L}$ satisfies the *detailed balance condition*, and the diffusion is *reversible*. Finally, we have that $\frac{1}{2}X^\mathcal{P}_\mathcal{S}$ is non-positive, i.e.,

$$\langle \frac{1}{2}X^\mathcal{P}_\mathcal{S}(f), f \rangle_P \leq 0$$

for all $f \in C^\infty_c(M)$. 


We refer the readers to §A.8 for the proof.

**Remark 5.4 (Carré du champ operator).** The generator $\mathcal{L}$ of any diffusion defines a *carré du champ* operator by

$$
\Gamma(f, h) = \frac{1}{2} (\mathcal{L}(fh) - f\mathcal{L}h - h\mathcal{L}f)
$$

over appropriate algebras of functions. These play an important role in the study of reversible diffusions (see [10] and references therein). Using (21), we see that the symmetric bracket $\mathcal{S}$ is in fact equivalent to the carré du champ operator $\Gamma$.

**Corollary 5.5.** For any $f, h \in C^\infty(M)$, the carré du champ operator of a $\mathcal{P}$-preserving diffusion is precisely the dissipative bracket generated by the noise $\Gamma(f, h) = \{f, h\}_S$.

The $L^2(\mathcal{P})$-symmetry of reversible Markov processes confers them important theoretical properties that are useful for example in the study of their convergence to equilibrium [10, 140]. However, they also form a restrictive class of diffusions that often have slow convergence properties [53, 138]. The decomposition of the generator above allows us to show that for appropriate transformations $\mathcal{R} : M \to M$, the generator of the $\mathcal{A}$-diffusion is *reversible up to* $\mathcal{R}$, which extends the notion of “reversibility up to momentum flip” of the Langevin diffusion in Euclidean space, usually associated with improved mixing properties [61, 152, 153].

**Corollary 5.6.** Let $\mathcal{R}$ be a target-preserving diffeomorphism, which is an $\mathcal{A}$-antimorphism and a $\mathcal{S}$-morphism, that is

$$
\mathcal{R}_* \mathcal{A} = -\mathcal{A}, \quad \mathcal{R}_* \mathcal{S} = \mathcal{S}.
$$

Then, the generator of the $\mathcal{A}$-diffusion (21) is *reversible up to* $\mathcal{R}$. That is, we have

$$
\langle f, \mathcal{L} h \rangle_\mathcal{P} = \langle \mathcal{L} \mathcal{R}^*_b f, \mathcal{R}^*_b h \rangle_\mathcal{P}, \quad \forall f, h \in C^\infty_c(M).
$$

**Example 5.7.** For instance, if $\mathcal{R}_* Y_i = \pm Y_i$, then $\mathcal{R}_* \mathcal{S} = \mathcal{S}$, and this is precisely what happens in the underdamped Langevin diffusion on phase space $(q, p)$ (see below), wherein $Y_i$ are proportional to $\partial_{p_i}$, and the momentum-flip $\mathcal{R} : (q, p) \mapsto (q, -p)$ flips the noise fields $\mathcal{R}_* Y_i = - Y_i$.

Combining the results from the previous sections, we have the following interpretations of the various components of measure-preserving diffusions:

$$
\begin{align*}
\text{d}Z_t = & \left( X^{\mu\mathcal{M}}_{\mathcal{A}} + X^\mathcal{A}_{H} \right) \, dt + \mathcal{P}^\mathcal{P}(\gamma) \, dt \\
& \quad + \left( -\frac{1}{2} Y_i(H) Y_i + \frac{1}{2} \text{div}_{\mu\mathcal{M}}(Y_i) Y_i \right) \, dt + Y_i \circ dW^i_t.
\end{align*}
$$

In particular, we note the following:
(i) $X_A^A$ (or $-Q\nabla H$) is the $p_\infty$-preserving ($X_A^A(p_\infty) = 0$) $A$-Hamiltonian vector field generated by an antisymmetric bracket $A$;

(ii) $X_M^\mu$ (or $\nabla \cdot Q$) is a generalisation of the modular vector field from Poisson mechanics, which preserves the volume measure $\mu_M$ and describes how the $A$-Hamiltonian vector fields $X_A^f$ distort the reference measure $\mu_M$, i.e., $X_M^\mu = 0$ iff $X_A^f$ preserves $\mu_M$ for all $f$.

(iii) When $X_M^\mu$ is added to $X_A^A$, the resulting vector field $X_P^A$ is $P$-preserving. On contractible manifolds such as $\mathbb{R}^n$, the Fokker–Planck current of any $P$-preserving diffusion can be written as $X_P^A$ for some $A$; otherwise, for (global) completeness, a topological obstruction term $P^\#(\gamma)$ parametrised by the $(n-1)^{th}$-twisted de Rham cohomology group $\gamma \in H_{dR}^{n-1}(M)$ must also be added by theorem 3.7. The resulting generator $X_P^A + P^\#(\gamma)$ is antisymmetric in $L^2(P)$. On compact oriented manifolds, this topological contribution can be parametrised by harmonic forms, as discussed in §4.

(iv) $\text{div}_{\mu_M}(Y_i)Y_i$ (or $\nabla \cdot D$ minus the Itô-to-Stratonovich correction) represents the distortion of the volume measure along the noise vector fields, and is usually dissipative;

(v) $-Y_i(H)Y_i$ (or $-D\nabla H$) is the rate of change of the target log-density along the noise fields.

(vi) The overall noise contribution (iv) + (v) is generated by the second-order “modular” operator $\frac{1}{2}X_P^A$, which is symmetric in $L^2(P)$.

6. Complete Recipe of Volume-Free $P$-preserving Diffusions

As noted in the introduction, obtaining a complete recipe of $P$-preserving diffusions allows practitioners to focus on the tuning of the parameters \{\mathcal{A}, \{Y_i\}\}, as well as its numerical implementation. Using the geometric formalism, we now discuss a particularly interesting class of parameters inspired by two classes of $P$-preserving diffusions that play a particularly central role in many applications, namely, the underdamped and overdamped Langevin processes, which are used for example to construct MALA and HMC respectively.

The overdamped Langevin process on $\mathbb{R}^n$ targets a measure of the form $P \propto e^{-H}dq$, and corresponds to the choices $Q = 0$ and $D = \text{arbitrary positive-definite constant matrix}$ in the Euclidean recipe (1):

\begin{equation}
    dZ_t = -D\nabla H + \sqrt{2D}dW_t.
\end{equation}

Since $D$ is a positive-definite contravariant tensor, we may think of it as a Riemannian co-metric. Thus, the drift $D\nabla H$ corresponds to a Riemannian gradient flow. On the other hand, the underdamped Langevin process evolves on the phase space $\mathbb{R}^n \times \mathbb{R}^n$ and preserve target measures of the form $P = \mu_H \propto e^{-H(q,p)}dqdp$. Starting from the Euclidean complete recipe, this is obtained by setting

\begin{equation}
    Q = -J = -\begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}, \quad D = \begin{pmatrix} 0 & 0 \\ 0 & C \end{pmatrix}
\end{equation}

where $J$ is the symplectic matrix and $C \in \mathbb{R}^{n \times n}$ is a positive semi-definite matrix \[153\] Sec. 2.2.3. This gives us the second-order Langevin process (also called the
underamped Langevin process)

\[ \text{div}_M(Y_i)Y_i = 0 \iff Y_i = \text{curl}_{\mu_M}(\mathcal{A}_i) + P^{\mu}(\alpha) \]

for which the terms involving the reference-measure \( \mu_M \) (we call this the ‘reference-measure drift’ in (25)) vanish. We refer to this subclass of \( \mathcal{A} \)-diffusions as \textit{volume-free} \( P \)-preserving diffusions.

While it is unclear how to even approach this problem from the Euclidean recipe/formalism, our geometric formalism provides an immediate characterisation of such processes in the case where the noise-fields \( (Y_i) \) are (pointwise) linearly independent. Indeed, in this case, we have

\[ \text{div}_{\mu_M}(Y_i)Y_i = 0 \iff Y_i = \text{curl}_{\mu_M}(\mathcal{A}_i) + P^{\mu}(\alpha) \]

and

\[ \text{curl}_{\mu_M}(\mathcal{A}_i) = 0 \iff \mathcal{A} = \text{curl}_{\mu_M}(\mathcal{V}) + P^{\mu}(\beta), \]

for some 3-vector field \( \mathcal{V} \in \mathfrak{X}^3(M) \), noise bi-vector fields \( \mathcal{A}_i \in \mathfrak{X}^2(M) \) (these are unrelated to the deterministic bi-vector field \( \mathcal{A}_i \)), and appropriate topological contributions \( \alpha \in H^{n-1}_d(M), \beta \in H^{n-2}_d(M) \) (see theorem B.1).

Hence, ignoring topological obstructions, volume-free \( P \)-preserving diffusions are characterised by parameters obtained through the rotationnels of higher-order tensors,

\[ \{\mathcal{A}_i, (Y_i)\} = \{\text{curl}_{\mu_M}(\mathcal{V}), (\text{curl}_{\mu_M}(\mathcal{A}_i))\}. \]

In particular, up to topological obstructions, such diffusions take the form

\[ dZ_t = X^{\text{curl}_{\mu_M}(\mathcal{V})}_t dt - \frac{1}{2} X^{\text{curl}_{\mu_M}(\mathcal{A}_i) \otimes \text{curl}_{\mu_M}(\mathcal{A}_j)}_t dt + \text{curl}_{\mu_M}(\mathcal{A}_i) \circ dW^i_t \]

and moreover, yield several geometric guarantees: first of all, the noise fields \( (Y_i) \) are automatically \( \mu_M \)-preserving (i.e., \( \text{div}_{\mu_M}(Y_i) = 0 \)) by construction, and secondly, any \( \mathcal{A} \)-Hamiltonian vector fields \( X^\mathcal{A}_f \) are also \( \mu_M \)-preserving for any \( f \in C^{\infty}(M) \), since by theorem B.3 we have

\[ 0 = \text{curl}_{\mu_M}(\mathcal{A})(f) = X^\mathcal{A}_{\mu_M}(f) = \text{div}_{\mu_M}(X^\mathcal{A}_f). \]

The latter property is crucial in HMC to avoid the appearance of Jacobians in the Metropolis-Hastings step, which are expensive to compute.

This suggests the following high-level strategy to sample using the volume-free \( P \)-preserving diffusions such that it maintains many of the geometric features that are key to the success of Hamiltonian-based Monte Carlo algorithms.
(1) Begin by considering the complete recipe of $P$-preserving diffusions
\[ dZ_t = (X^P_A + P^\sharp(\gamma) + \frac{1}{2} \text{div}_P(Y_i)Y_i)dt + Y_i(Z_t) \circ dW^i_t. \]
In general, it is not possible to obtain a computationally tractable expression for the solution to this system, since the solution must possess some symmetry for it to be tractable, whereas the target measure typically do not possess such symmetries. This leads us to the next step.

(2) Decompose the target $P$ as $P \propto e^{-H} \mu_M$, where $\mu_M$ is an appropriate reference measure, for which tractable $\mu_M$-preserving flows can be obtained. Hence, $\mu_M$ is usually an invariant measure, such as the Lebesgue or Haar measure, or a simple probability measure, such as a Gaussian measure. The complexity of the target $P$ is then entirely contained within its density $e^{-H}$.

We thus have the expression
\[ dZ_t = (X^H_A - \frac{1}{2} Y_i(H)Y_i)dt + (X^\mu_M + \frac{1}{2} \text{div}_{\mu_M}(Y_i)Y_i)dt + P^\sharp(\gamma)dt + Y_i \circ dW^i_t, \]

(3) In order to reduce the complexity of the target density $e^{-H}$, we further split it into simpler components, $e^{-H} = \prod_j e^{-H_j}$. This is one of the important benefits associated to the lifting procedure used in HMC and the underdamped Langevin process, wherein the target density is complex, but its lift typically decomposes nicely into a potential $V(q)$ and kinetic $T(p)$ term, both of which are simpler to handle in the lifted space since $V$ is $p$-independent and $T$ is $q$-independent. Hence, when such simpler components do not exist, we must lift the process to some phase space, i.e., vector bundle, over $M$ where such decompositions exist.

(4) Split the diffusion further into an $L^2(P)$-symmetric process
\[ dZ^S_t \equiv -\frac{1}{2} \sum_j Y_i(H_j)Y_i dt + \frac{1}{2} \text{div}_{\mu_M}(Y_i)Y_i dt + Y_i \circ dW^i_t, \]
and an $L^2(P)$-antisymmetric, deterministic process
\[ dZ^A_t \equiv \left( \sum_j X^H_{A_j} + X^\mu_M + P^\sharp(\gamma) \right)dt. \]
Hereafter, we will discard the topological obstruction term $P^\sharp(\gamma)$ for simplicity, as they are not necessary for measure-preservation.

(5) Restrict the reversible component to volume-free processes, so that we get
\[ dZ^S_t = -\frac{1}{2} \sum_j X^\text{curl}_{H_j}(\mu_M) \otimes \text{curl}_{H_j}(\mu_M) \circ dW^i_t, \]
which ensures that the noise vector fields $Y_i = \text{curl}_{\mu_M}(A_i)$ are volume-preserving, similar to the Langevin system. On $M = \mathbb{R}^n$, this can be implemented with an explicit integrator, as shown in [29] and on more general manifolds $M$, the process can be lifted to a vector bundle over $M$ and choosing the noise-fields to be vertical, the process will evolve purely on the fibres (which are vector spaces), where we can integrate this explicitly.
(6) For the irreversible component, setting $\mathcal{A} = \text{curl}_{\mu_M}(\mathcal{V})$, the deterministic process simplifies to
\[
\frac{dZ_t}{dt} = \sum_j X_{H_j}^{\text{curl}_{\mu_M}(\mathcal{V})},
\]
which can be implemented with a palindromic splitting integrator [130, 77], that approximates the $\mathcal{P}$-preserving flow of $X_{H_j}^{\text{curl}_{\mu_M}(\mathcal{V})}$ with the composition of the flows of $X_{H_j}^{\text{curl}_{\mu_M}(\mathcal{V})}$. Importantly, as discussed above, the choice $\mathcal{A} = \text{curl}_{\mu_M}(\mathcal{V})$ guarantees that the splitting integrator will be volume-preserving. Essentially, the splitting method used to compute the irreversible process simplifies the implementation by decomposing the complicated target $e^{-H_{\mu_M}}$ into simpler targets $e^{-H_{\mu_M}}$, for which the corresponding flows are easier to construct, while still ensuring that the resulting numerical integrator is $\mu_M$-preserving. Here, again, if $H$ is too complex and does not have a sufficiently nice decomposition, it will be necessary to lift the process to an appropriate phase space where such decompositions exist. In general, it is desirable to choose the potentials $\{\mathcal{V}_i(\mathcal{A}_i)\}$ that share the symmetries of the reference measure, in order for the tensor fields $\text{curl}_{\mu_M}(\mathcal{V})$ and $\text{curl}_{\mu_M}(\mathcal{A})$ to inherit these symmetries.

**Example 6.1 (Shadows).** Choosing $\mathcal{A}$ to be a Poisson structure with invariant measure $\mu_M$ (such as those discussed in [44, 159, 52]) further ensures that the splitting integrator used to integrate the irreversible deterministic component will have a modified energy, called the shadow Hamiltonian, as a result of the Jacobi identity. In other words, the numerical integrator will itself be a $\mathcal{A}$-Hamiltonian vector field with respect to the shadow Hamiltonian, and this feature is important to the success of HMC (see [105, 94, 154, 92, 142, 30]). When the Poisson structure is constructed on a vector bundle over $M$, such as the cotangent bundle, and the noise fields are chosen to be vertical, we obtain a natural generalisation of [7], where an irreversible HMC algorithm on compact Lie groups was obtained, following the SOL-HMC construction in [139] (see also §9).

In general, the Brownian motion $dW^i_t$ (resp. its Riemannian generalisation, discussed below) on $\mathbb{R}^n$ (resp. on a Riemannian manifold) only preserves the Lebesgue measure $dx$ (resp. the Riemannian measure). By choosing $H = 0$ and therefore $P = \mu_M$, the diffusion (26) reduces to
\[
dZ_t = \text{curl}_P(\mathcal{A}) \circ dW^i_t,
\]
which may be thought of as the general class of $P$-preserving Brownian motions, wherein the Euclidean Brownian motion $dW^i_t$ is directed along $P$-preserving vector fields $\text{curl}_P(\mathcal{A})$, to obtain a general measure-preserving Brownian motion.

7. **Itô Diffusions with Riemannian Brownian Noise**

We now consider noise processes that are driven by Riemannian Brownian motion, which have powerful ergodic properties. We say that a diffusion process is non-degenerate when its generator is elliptic, and in this case, we can find a Riemannian metric $\mathcal{M}$ for which the generator takes the form
\[
\mathcal{L} = X + \frac{1}{2} \Delta,
\]
for some drift $X \in \mathfrak{X}(\mathcal{M})$.
where $\frac{1}{2}\Delta$ is the Laplace-Beltrami operator associated with the metric $\mathcal{M}$ (see \cite{90}). The diffusion $B_t$ generated by $\frac{1}{2}\Delta$ on $\mathcal{M}$ is called the Riemannian Brownian motion (see \cite{89}), and such processes are used for instance in the construction of stochastic gradient descent (SGD). To get a glimpse of how this noise process is related to the Stratonovich noise discussed earlier, note that when the dissipative bracket $\mathcal{S} \equiv Y_i \otimes Y_i \in \mathcal{X}^2(\mathcal{M})$ is positive definite, it defines a Riemannian co-metric on $\mathcal{M}$. Conversely, given a Riemannian metric $\mathcal{M}$ on $\mathcal{M}$, there always exists a local expansion of the co-metric $\mathcal{M}^{-1}$ in terms of a finite set of vector fields $(Y_i)$, as $\mathcal{M}^{-1} = Y_i \otimes Y_i$, since $\mathcal{M}^{-1}$ is positive definite (this is analogous to taking the square-root of a positive definite matrix on $\mathbb{R}^n$).

The following theorem gives a full characterisation of $P$-preserving diffusions generated by (27) (see §A.9 for the proof).

**Theorem 7.1.** Let $\mathrm{vol}$, $\nabla$ and $\nabla \cdot$ be the Riemannian measure, gradient and divergence respectively. Any $P \propto \rho_{\infty} \mathrm{vol}$-preserving diffusion generated by (27) takes for some $\mathcal{A} \in \mathcal{X}(\mathcal{M})$, the form (up to the usual topological obstruction term)

$$
\begin{align*}
\mathrm{d}Z_t &= -\mathbf{X}^\mathcal{A}_{\log \rho_{\infty}}(Z_t) \mathrm{d}t - \nabla \cdot \mathbf{A}(Z_t) \mathrm{d}t \\
&+ \frac{1}{2} \nabla \log \rho_{\infty}(Z_t) \mathrm{d}t + \mathrm{d}B_t \\
&= \text{Riemannian gradient flow} + \text{Riemannian Brownian motion} + \text{reversible Riemannian overdamped Langevin system}
\end{align*}
$$

(28)

We defer the discussion on the ergodicity of (28) on paracompact manifolds in \cite{110}. In the reversible case $\mathcal{A} = 0$, the diffusion (28) gives us precisely the Riemannian overdamped Langevin equation, used to construct the Riemann Metropolis-adjusted Langevin algorithm (MALA) when the Riemannian metric is obtained from an information divergence (see \cite{68, 117}). On the other hand, the case $\mathcal{A} \neq 0$ is also of interest to us as it is well-known that the existence of an irreversible component can accelerate convergence to the target distribution, as demonstrated in \cite{89, 53, 145} (a detailed analysis of the optimal drift for constant $\mathcal{A}$ is provided in \cite{109}). Alternatively, reversible overdamped Langevin systems ($\mathcal{A} = 0$) with appropriate choices of Riemannian metric $\mathcal{M}$ can also lead to accelerated convergence relative to the overdamped Langevin process (23), as shown in \cite{1}.

**Remark 7.2 (Reference Measures).** We point out that the Riemannian measure associated to the metric of the generator is sometimes not an appropriate choice of reference measure. This has in fact caused considerable confusion in the statistical literature when a target on Euclidean space is expressed in terms of the Riemannian measure instead of the Lebesgue measure \cite{34, 115, 161}. In that case, denoting by $\rho_M$ the density of $P$ with respect to an appropriate reference measure $\mu_M$ and $\rho_{\infty}$ the density associated with the Riemannian measure $\mu$, we can simply use the relation $\log \rho_{\infty} = \log \rho_M - \log \frac{\mathrm{dvol}}{\mu_{\infty}}$ to convert (28) into a corresponding expression based on the measure $\mu_M$. For example on Euclidean space, it is well-known that the Riemannian Brownian motion $B_t$ can be expressed as $\mathrm{d}B_t = \sqrt{\mathcal{M}^{-1}} \mathrm{d}W_t - \frac{1}{2} \mathcal{Y}_{\mathcal{M}} \mathrm{d}t$, where $\mathcal{Y}_{\mathcal{M}} \equiv \mathcal{M}^{ij} \mathcal{Y}_i \mathcal{Y}_j = \mathcal{M}^{ij} \partial_i \log \sqrt{\mathcal{M}} - \partial_i \mathcal{M}^{ij}$ and $W_t$ is the standard Euclidean Brownian motion. Further, if $\mu_M = \mathrm{dx}$, then $\mathrm{dvol} / \mu_{\infty} = \sqrt{\mathcal{M}}$ and together with the explicit expression for $\mathrm{d}B_t$, we can use this to express (28) in terms of the local Lebesgue density, as in \cite{161}. One should note however that $\mu_M = \mathrm{dx}$ is not a
meaningful measure on general manifolds and therefore this expression only makes sense on Euclidean space.

In local charts, one can also recover the Riemannian overdamped Langevin system directly from our \( A \)-diffusion \( \mathcal{A} \) as we show below. First, let \( \{Y_i\} \) be a family of vector fields on \( M \) such that \( S \equiv Y_i \otimes Y_i \) is a positive definite tensor field. We then set \( M \equiv S^{-1} \), which defines a Riemannian metric tensor. Now taking the reference measure \( \mu_M \) to be the Riemannian measure \( \text{vol} \) (locally, \( \text{vol} = \sqrt{|M|} \, dx \) where \( |M| \) denotes the local determinant of \( M \)), the \( A \)-diffusion \( \mathcal{A} \) with \( A = 0 \) becomes

\[
dZ_t = -\frac{\beta}{2} Y_i(H) Y_i \, dt + \frac{1}{2} \text{div}_{\text{vol}}(Y_i) Y_i \, dt + Y_i \circ dW_i^t.
\]

For the first term, we have \( Y_i(H) Y_i = X_H^{-1} = \nabla H \), so it is the Riemannian gradient of \( H \). In local coordinates, the second term reads

\[
\frac{1}{2} \text{div}_{\text{vol}}(Y_i) Y_i^k = \frac{1}{2} \frac{\partial}{\partial x^j} \left( \sqrt{|M|} Y_i^j \right) Y_i^k
= \frac{1}{2} \frac{\partial}{\partial x^j} \left( \sqrt{|M|} Y_i^j Y_i^k \right) - \frac{1}{2} Y_i^j \frac{\partial}{\partial x^j} Y_i^k,
\]

and the random noise terms are related by the Stratonovich-to-Itô correction

\[
\underbrace{Y_i^k \circ dW_i^t}_{\text{Stratonovich noise}} = \underbrace{\frac{1}{2} Y_i^j \frac{\partial Y_i^k}{\partial x^j} \, dt}_{\text{Stratonovich-to-Itô correction}} + \underbrace{Y_i^k \, dW_i^t}_{\text{Itô noise}}.
\]

Hence putting this together, we have

\[
\frac{1}{2} \text{div}_{\text{vol}}(Y_i) Y_i^k \, dt + Y_i^k \circ dW_i^t = \frac{1}{2} \frac{\partial}{\partial x^j} \left( \sqrt{|M|} Y_i^j Y_i^k \right) \, dt + Y_i^k \, dW_i^t,
\]

which is precisely the local expression for the Riemannian Brownian motion \( dB_t \) \[85\]. Thus, in local charts, \( \mathcal{A} \) becomes

\[
dZ_t = -\frac{\beta}{2} \nabla H \, dt + dB_t,
\]

which is exactly the Riemannian overdamped Langevin system.

**Remark 7.3 (Riemannian Brownian Motion from the Orthonormal Frame Bundle).** We show here that the Riemannian Brownian motion can also be obtained globally as a projection of a Stratonovich diffusion defined on the orthonormal frame bundle. Specifically, if we define the canonical horizontal vector field \( L_i \) on the orthonormal frame bundle \( \pi_O : O(M) \to M \), then the diffusion \( dO_t = L_i \circ dW^i_t \) reduces to the Riemannian Brownian motion \[90\] theorem 4.2. Moreover \( L_i(\pi_O^* H) L_i \) is \( \pi_O \)-related to \( \nabla H \), as follows from equations (4.12) and (4.22) in \[90\]. Indeed, locally \( L_i = e_i^s \partial_q - \Gamma^s_{ab} e_i^a \partial_e e_b^s \) where \( \{e_s\} \) is an orthonormal frame, so \( L_i(\pi_O^* H) L_i = e_i^s \partial_q (H) e_s^a \partial_e e_b^a = M^{rs} \partial_q (H) \partial_r \). Hence the Riemannian overdamped Langevin process \( dQ_t = -\frac{\beta}{2} \nabla H \, dt + dB_t \), is the projection under \( \pi_O \) of the Stratonovich diffusions \( dQ_t = -\frac{\beta}{2} L_i(\pi_O^* H) L_i \, dt + L_i \circ dW^i_t \).
8. Deterministic Flow of Measure-Preserving Diffusions on the Space of Volume Measures

In this section, we describe the rate of change of functionals along the diffusion process. The rate of change of a curve of volume measures $\mu_t$ along a diffusion process $Z_t$ is given by the forward Kolmogorov equation,

$$\frac{\partial \mu_t}{\partial t} = \mathcal{L}^* \mu_t.$$ 

In particular, if $Z_t$ is an arbitrary $P$-preserving diffusion, combining (13) and theorem 3.7, we find that the equation

$$\frac{\partial \mu_t}{\partial t} = \text{div} \mu_t \left( -\text{curl} P(\mathcal{A}) + \frac{1}{2}(\text{div} \mu_t(Y_i) - \text{div} P(Y_i))Y_i \right) \mu_t$$

describes the evolution over the space of smooth measures of $\mu_t$ towards the stationary distribution $P$. Decomposing at each $t$ the target $P$ with respect to the reference measure $\mu_t$, as in (11), and using the fact $\text{curl} \circ \text{curl} = 0$, we can simplify this expression to

$$\frac{\partial \mu_t}{\partial t} = \text{div} \mu_t \left( \frac{1}{2} X^S \log \frac{dP}{d\mu_t} - X^A \log \frac{dP}{d\mu_t} \right) \mu_t - dP(\mu_t)(\mu_t^0(\gamma)) \mu_t.$$ 

Let us for the moment ignore the topological obstruction for simplicity. Observe that $\mu_t$ satisfies the continuity equation

$$\frac{\partial \mu_t}{\partial t} + \text{div} \mu_t \left( \frac{1}{2} X^S \log \frac{dP}{d\mu_t} - X^A \log \frac{dP}{d\mu_t} \right) \mu_t = 0.$$ 

Hence, the rate of change of KL divergence along the curve $\mu_t$ is

$$\frac{d}{dt} \text{KL}(\mu_t \| P) = - \int \text{div} P \left( \frac{1}{2} X^S \log \frac{dP}{d\mu_t} - X^A \log \frac{dP}{d\mu_t} \right) \mu_t,$$

and if Stokes' theorem hold, we can further write (recall the notation (18))

$$\frac{d}{dt} \text{KL}(\mu_t \| P) = - \frac{1}{2} \int \left\{ \log \frac{dP}{d\mu_t}, \log \frac{dP}{d\mu_t} \right\} S \mu_t.$$ 

Since $S$ is a dissipative bracket and $\mu_t$ is a smooth positive measure, this integral is non-negative for all $t$, and it follows that

$$\frac{d}{dt} \text{KL}(\mu_t \| P) \leq 0,$$

in concordance with the Euclidean case, see for example [120]

More generally, consider a functional $F$ on the space of smooth measures. Important families of such functionals include the linear functionals

$$F_f(Q) \equiv \langle f, Q \rangle = \int fQ,$$

for some $f \in C^\infty(M)$, and the functionals

$$F^P_h(Q) \equiv \int h \left( \frac{dQ}{dP} \right) Q,$$

parametrised by a choice of function $h : \mathbb{R} \rightarrow \mathbb{R}$, which include the KL divergence and other functionals that arise in a wide range of applications [96, 119, 128, 85].

\[that is \int \text{div} \mu_t \left( \frac{1}{2} X^S \log \frac{dP}{d\mu_t} - X^A \log \frac{dP}{d\mu_t} \right) \mu_t = 0\]
The functional derivatives $\frac{\delta F}{\delta Q}$ with $F = F_f$ and $F^P_h$ are $f$ and $h \left( \frac{\delta Q}{\delta P} \right)$ respectively. For any bracket $\mathcal{B}$, we define the integral bracket on the space of measures by

$\{f, h\}_\mathcal{B}(Q) \equiv \int \{f, h\}_\mathcal{B} Q,$

provided the integral converges (for example, $f$ or $h$ is compactly supported). The following proposition shows that the integral thermodynamic bracket associated to the diffusion characterises the rate of change of $F$ along the process (see §A.10 for the proof). It can be used to optimize the brackets in the measure-preserving diffusion for the given task, for example to improve the decay of a statistical divergence (see e.g. [135]) along the process to speed-up convergence to equilibrium.

**Proposition 8.1.** Let $F$ be a functional on the space of volume measures, and suppose $\frac{\delta F}{\delta Q} \in C^\infty_\text{c}(M)$ (or more generally that Stokes’ theorem holds). The rate of change of $F$ along the $P$-preserving diffusion is then given by

$$
\frac{d}{dt} F(\mu_t) = \left\{ \log \frac{dP}{d\mu_t}, \frac{\delta F}{\delta \mu_t} \right\}_{\mathcal{T}} + \left\{ \frac{d\mu_t}{dP}, \mu_t^*(\gamma) \left[ \frac{\delta F}{\delta \mu_t} \right] \right\}_{\mu_t}
$$

where $\mathcal{T}$ is the thermodynamic bracket $\mathcal{S}/\sqrt{2} - \mathcal{A}$, and $\gamma$ the topological obstruction.

9. Underdamped Langevin Diffusions on Manifolds

As discussed in §6, an important feature common to both the underdamped and overdamped Langevin processes is the fact that they are both measure-preserving despite having no explicit reference measure contribution. Therein we have derived the complete characterisation of these Langevin-like measure-preserving systems.

In this section, we will introduce another perspective regarding the underdamped Langevin process (24), and use this to construct irreversible Langevin-based MCMC samplers on manifolds. The idea is as follows. Since the underdamped Langevin system evolves on a vector bundle $\pi : \mathcal{F} \to M$ and we want the noise process to live entirely in the vertical direction, we can ask what are the measures $\mu_F$ on $F$ for which all vertical vector fields are $\mu_F$-preserving, so that any choice of vertical noise gives rise to a volume-free measure-preserving diffusion. This motivates the notion of a Langevin pair, defined as a pair $(\mathcal{A}, \mu_T)$ such that

- for any function $f$, $X^\mathcal{A}_f$ is $\mu_T$-preserving
- $\mu_T$ is horizontal, i.e., $L_Y \mu_T = 0$ for any vertical vector field $Y$.

The $\mathcal{A}$-diffusion generated by a Langevin pair $(\mathcal{A}, \mu_T)$ recovers the Langevin diffusions (24) locally for any choice of vertical noise fields $(Y_i)$, with the deterministic Hamiltonian dynamics on $\mathbb{R}^n \times \mathbb{R}^n$ therein replaced by a more general $\mathcal{A}$-Hamiltonian vector field on $\mathcal{F}$.

As we will see below, when $\mathcal{F} = TM$ is the tangent bundle over a Riemannian manifold, choosing the noise to be vertical ensures that when $(\mathcal{A}, \mu_{TM})$ is a Langevin pair and the Hamiltonian corresponds to a simple mechanical system, $H \equiv \pi^* V + \frac{1}{2} \| \cdot \|^2$ (here $\| \cdot \|$ is the Riemannian norm), the thermostat process becomes an OU process on the fibres, for which there is an explicit solution, and furthermore preserves the Gaussian distribution $e^{-\frac{1}{2} \mathcal{M}(v, v)}$ on the fibres defined with respect to the Riemannian metric $\mathcal{M}$. An important example of a Langevin pair and target $\mu_{TM} \equiv e^{-\pi^* V - \frac{1}{2} \| \cdot \|^2} \mu_{TM}$ arises when the target $P$ on $M$ is expressed in terms of the Riemannian measure, $P = e^{-V} \text{vol}$. In this case, if $\omega^n$ denotes the
Riemannian symplectic measure (associated to the symplectic structure \( \omega_\flat \equiv \flat^*\omega \) with \( \flat \) the musical isomorphism), which in local tangent-lifted coordinate reads \( \omega_\flat^a = |\mathcal{M}|dqdv \), then the pushforward of \( \mu_H \) with \( \mu_{TM} = \omega_\flat^a \) is simply the target \( \pi_*\mu_H = P \), so that any samples generated from a \( \mu_H \)-preserving process are transported under \( \pi \) to samples from \( P \). Denoting by \( \mathcal{V} \) the vertical lift of vector fields on \( \mathcal{M} \) (which maps vector on \( \mathcal{M} \) to vectors on \( TM \), see proof in §A.11 for the formal definition), we have the following result.

**Theorem 9.1.** Suppose \((\mathcal{A}, \mu_{TM})\) is a Langevin pair. If we choose the noise fields to be the vertical fields \( Y_i \equiv \mathcal{V} \circ X_i \circ \pi \) for \( X_i \in \mathfrak{X}(\mathcal{M}) \), then the \( \mathcal{A} \)-diffusion generated by \( e^{-H}\mu_{TM} \) with \( H \equiv \pi^*\mathcal{V} + \frac{1}{2}||\cdot||^2 \), reads

\[
\frac{d(q_t, v_t)}{dt} = X^\mathcal{A}_{H}(q_t, v_t)dt - \frac{1}{2} \langle X_i(q_t), v_t \rangle q_t \mathcal{V}(X_i(q_t))dt + \mathcal{V}(X_i(q_t)) \circ dW_t,
\]

where \( \langle u, v \rangle_q \equiv \mathcal{M}(u, v) \) is the Riemannian inner product at \( q \in \mathcal{M} \), or in tangent-lifted coordinates,

\[
\frac{d(q_t, v_t)}{dt} = \left( X^\mathcal{A}_{H}(q_t, v_t) - \frac{1}{2}M(q_t)v_t \right)dt + \sigma(q_t) \circ dW_t,
\]

where \( M(q)v = M(q)_{ij}v^j\partial_{v^i} \equiv (\sigma^\top\mathcal{M}(q))_{ij}v^j\partial_{v^i}, \quad \sigma \equiv \sigma_{ij}\partial_{v^i} \equiv (X_i)^j\partial_{v^i}, \quad \text{and} \quad \mathcal{M}_{ij}(q) = \langle \partial_{v^i}, \partial_{v^j} \rangle_q \).

In particular \((\Pi, \omega^n)\) is a Langevin pair, where \( \Pi \) is the Poisson bi-vector field associated to \( \omega_\flat \).

When \( \mathcal{F} \) is isomorphic to \( TM \), for example \( \mathcal{F} = T^*\mathcal{M} \), then we can use the isomorphism to rewrite (30) over \( \mathcal{F} \). In particular when \( \mathcal{M} = \mathbb{R}^n \) and \( T(q, v) = \frac{1}{2}v^\top Mv \), using the musical isomorphism, the SDE (32) becomes the Langevin dynamics on phase space, as seen in [31] (with \( \sqrt{C} \equiv \mathcal{M}\sigma, C \equiv \mathcal{M}\sigma^\top\mathcal{M} \))

\[
\frac{dQ_t}{dt} = M^{-1}P_tdt, \quad \frac{dP_t}{dt} = -\nabla V(Q_t)dt - \frac{1}{2}C(Q_t)M^{-1}(Q_t)P_tdt + \sqrt{C(Q_t)}dW_t,
\]

where now, the definition \( M \equiv \sigma^\top\mathcal{M} \) in theorem 9.1 plays the role of the “fluctuation-dissipation relation” which ensures that the target \( \propto e^{-H}dqdp \) is preserved. We thus see that, as claimed, (31) is the manifold generalisation of the usual Langevin SDE, where the noise vector fields \( X_i \) represent the columns of the “vertical matrix” \( \sigma \), which only introduces randomness along the fibres (velocity), and \( \langle X_i(q_t), v_t \rangle_q \) describes the rate of change of the kinetic energy along the noise. On \( \mathcal{F} = \mathbb{R}^n \times \mathbb{R}^n \), another example of a Langevin pair consists in choosing \( \mathcal{A} \) to be a constant anti-symmetric matrix (which is Poisson but not necessarily symplectic), and \( \mu_{\mathcal{F}} \) the Lebesgue measure \( dqdp \). It would be interesting to analyse the optimal properties of a subclass of these Langevin processes as proposed in [109].

We can now proceed to build various irreversible, Langevin-based MCMC schemes (which we abbreviate as iLMCMC) in a similar fashion to [34 139 49].

### 9.1. iLMCMC Algorithm

Using vertical noise fields, we see that (31) naturally decomposes into a Hamiltonian part and a vertical part which remains within the initial fibre, and thus only shifts the velocity (i.e., replaces the HMC heat bath). We split (31) into an \( \mathcal{A} \)-Hamiltonian part on \( TM \)

\[
\frac{dz}{dt} = X^\mathcal{A}_{H}(z),
\]
and an OU process within the tangent fibres $T_qM$ (since the vertical lift is an
isomorphism $T_q(T_qM) \cong T_qM$)

$$\dot{q} = 0, \quad \dot{v}_t = -\frac{\beta}{2} \langle X_i(q), v_t \rangle_q X_i(q)dt + X_i(q) \circ dW_t,$$

which locally has the form

$$\dot{q} = 0, \quad \dot{v}_t = -\frac{\beta}{2} M(q)v_t dt + \sigma(q) \circ dW_t,$$

and preserves the Gaussian $\propto e^{-\frac{1}{2}(v,v)^T}dv = \mathcal{N}(0, M^{-1}(q))$. Thus, by choosing
vertical noise fields $Y_t$ and a Langevin pair $(\mathcal{A}, \mu \sigma)$ in the general $\mathcal{A}$-diffusion, we obtain a diffusion which splits naturally into an $\mathcal{A}$-Hamiltonian vector field and a
tractable OU-process in the fibres, as with the Euclidean case.

Below, we consider the bracket $\mathcal{A} = \Pi$ associated with the Riemannian symplec-
tic structure, that is $X^H_f$ is the Hamiltonian vector field of $f$ with respect to $\omega_q$, and
its geodesic integrators, and then consider the special case when $M$ is a Lie
group, where we recover a modified version of the algorithm presented in [7] that is
cheaper to compute.

9.2. iLMCMC with Geodesic Integrators on Embedded Manifolds. Suppose that $\iota : \mathcal{M} \hookrightarrow \mathbb{R}^k$ is an embedded manifold, equipped with a Riemannian
metric that is defined by restricting the Euclidean metric to $\mathcal{M}$. We assume that we have (1) a tractable expression for the geodesic flow $\Phi^t$ of the kinetic energy $T \equiv \frac{1}{2}||v||^2$, (2) a $C^1$-extension $W$ of the potential energy $V$ in the coordinates of the
embedding, and (3) that the Riemannian metric corresponds to that used to define the
reference measure of $P$ - otherwise we need to add a Radon–Nykodym term in
our Hamiltonian. If the geodesic flow is computationally intractable, convenient al-
ternatives include the Riemannian integrators [10], or RATTLE with reversibility
check [111, 106]. Then we can apply a geodesic integrator which approximates
by a composition of geodesic flow $\Phi^t$, and vertical gradient flow generated by $X^H_V$, whose integral curve starting from $(q_0, v_0) \in T\mathbb{R}^k|\mathcal{M}$ reads

$$q(t) = q_0 \quad v(t) = v_0 - t \text{hor} (\nabla_{q_0} W),$$

where $\nabla_{q_0} W$ is the Euclidean gradient and hor is the orthogonal projection onto
the tangent space of $\mathcal{M}$. Similarly, to implement [111], we need the noise vector fields $X_i$ to be expressed in the coordinates of the embedding: that is, each noise field $X_i$ is given by a vector field $b_i = (b^1_i, \ldots, b^k_i)$ on $T\mathbb{R}^k|\mathcal{M}$ (i.e., $\partial \circ X_i = b_i \circ \iota$). Then $b_i$ defines the $i^{th}$ column of the matrix $\sigma$ and the process [111] is $\partial_{q,t}$-related to the following process on $\mathbb{R}^k$ ($\cdot, \cdot$ is the dot product)

$$dy_t = -\frac{\beta}{2} b_i(q) \cdot y_t b_i(q) dt + \sigma(q) dW_t.$$

Note that our potential energy does not include a $\log |\mathcal{M}|$ term, unlike the geo-
desic MCMC of [115]. Indeed, as we discussed in the previous chapter, this terms
does not give rise to a meaningful potential energy on manifolds. In the very special
case in which $\mathcal{M} = \mathbb{R}^k$ and we have fixed a coordinate system (so $\mathbb{R}^k$ is no longer
a manifold), then we can add the “correction term” $\log |\mathcal{M}|$ to the potential energy
in order to ensure that the algorithm generates samples from $e^{-V}dq$ rather than

\footnote{with $T_q\mathcal{M} \cong \mathbb{R}^n$ using the local basis, $M(q) \equiv \sigma(q)\sigma^T(q)\mathcal{M}(q)$ where $\sigma_{ji}(q) \equiv (X_i(q))_j$.}
$e^{-V \text{vol}}$, since typically, distributions on the Euclidean space are expressed in terms of the Lebesgue measure (see also [79]).

9.3. iLMCMC on Lie Groups. Suppose now that the configuration space $\mathcal{M} = \mathcal{G}$ is a Lie group equipped with a left-invariant metric, $(\theta^i)$ is a set of Maurer–Cartan 1-forms, and $\mathcal{S}$ is the symplectic manifold $\mathcal{G} \times \mathfrak{g}$ [13]. The identity element of $\mathcal{G}$ will be denoted by 1.

Let $v^i : \mathcal{G} \to \mathbb{R}$ defined by $v^i(\xi) = \theta^i(\xi)$ be the coordinates on $\mathcal{G}$, associated to the basis $(\xi_i)$ of the Lie algebra $\mathfrak{g}$ dual to the Maurer–Cartan 1-forms (i.e., $\theta^i_\xi(\xi_j) = \delta^i_j$). Since $T(\mathcal{S} \times \mathcal{G}) = T\mathcal{G} \oplus T\mathfrak{g}$, the vector fields on $\mathcal{S} \times \mathcal{G}$ can be expanded as $\dot{X} = a^i e_i + b^i \partial_{v^i}$, where $\partial_{v^i} \in \Gamma(T\mathfrak{g})$ and $e_i$ is the left-invariant vector field dual to $\theta^i$. In [7], where the authors first derive an irreversible MCMC algorithm on Lie groups, the Hamiltonian fields were chosen to be of the form $U = \delta \mathcal{H}_1 \otimes \theta^1$ for some noise potentials $U_i : \mathcal{G} \to \mathbb{R}$. Here, we will instead choose the noise fields to be $Y_i = \partial_{v^i}$ to make the computation of the OU process cheaper as we shall see (we could also have $Y_i = f_i(g) \partial_{v^i}$). It follows from theorem [9.1] that $\text{div} \mathcal{H}_1 Y_i = 0$ since $\partial_{v^i} = \nabla(\xi_i)^T$. Then, taking the kinetic energy $T \equiv \frac{1}{2} \mathcal{M}_{ij} \theta^i \otimes \theta^j$ on $\mathfrak{g}$ associated to the left-invariant metric with matrix $\mathcal{M}$, (31) becomes

$$\dot{q} = v^i e_j(q_t), \quad \text{dv}_t = \text{ad}^\mathfrak{g}_{v^i} v dt - \frac{1}{2} \mathcal{M}_{jk}(V)(q_t) \dot{\xi}_k dt - \frac{\beta}{2} v^i dt + dW_t,$$

where $(q_t, v_t) \in \mathcal{G} \times \mathfrak{g}$. The Euler-Arnold term describes the geodesic motion of a Riemannian metric with symmetries (in this case left invariance), and vanishes if the inner product on $\mathfrak{g}$ is ad-invariant [82, 131]. In particular on SU(3), the diffusion splits into the transition steps used in the Hybrid Monte Carlo simulation for lattice QCD, with the OU process replacing the momentum heat bath. In Euclidean space, we have $e_j = \xi_j = \partial_{\xi_j}$, and we recover the second order Langevin equation [159, 49].

It is particularly nice that the Ornstein-Uhlenbeck process $dv_t = -\frac{1}{2} v^i dt + dW_t$ on $\mathfrak{g}$ has an explicit solution given by

$$v_{t+h} = e^{-\frac{1}{2} h} v_t + \int_t^{t+h} e^{-\frac{1}{2} (t+h-s)} dW_s,$$

with transition probability

$$p(v_0, v) = \sqrt{\frac{1}{(2\pi)^n (1 - e^{-\beta h})}} \exp \left( -\frac{1}{2 (1 - e^{-\beta h})} \| v - e^{-\frac{1}{2} h} v_0 \|^2 \right).$$

Hence, given an initial sample $(g_0, v_0)$, we obtain an irreversible MCMC algorithm on Lie groups by implementing the following steps:

---

5In fact we can check this directly without relying on local coordinates: writing the left Haar measure as $\Theta \equiv \theta^1 \times \cdots \times \theta^n$, we have

$$\mathcal{L}_{\partial_{v^i}} \omega^\mathfrak{g} = (\mathcal{L}_{\partial_{v^i}} dv) \wedge \pi^\ast \Theta + dv \wedge (\mathcal{L}_{\partial_{v^i}} \pi^\ast \Theta).$$

Now $\mathcal{L}_{\partial_{v^i}} dv = d\mathcal{L}_{\partial_{v^i}} v^j = d\delta_{v^j} v^i = d\delta_{v^i} v^i = 0$. Then we have $\mathcal{L}_{\partial_{v^i}} \pi^\ast \Theta = 0$, since the flow $\Phi_\ast \partial_{v^i}$ is only non-trivial in the vertical direction. Indeed its flow is $\Phi_\ast (g, v) = (g, v^i, \ldots, v^i + t, \ldots, v^n)$ so

$$\left(\mathcal{L}_{\partial_{v^i}} \pi^\ast \Theta\right)(g, v) = \frac{d}{dt} |_{t=0} (\Phi_t^\ast (g, v) \pi^\ast \Theta) = \frac{d}{dt} |_{t=0} \left( (\pi \circ \Phi_t (g, v))^\ast \Theta \right) = 0,$$

since $\pi \circ \Phi_t (g, v) = g$ is independent of $t$. 

---
(1) Solve the OU process exactly until time \(h\) by sampling
\[
\nu^* \sim \mathcal{N}\left(e^{-\frac{1}{2}h}\nu_0, (1-e^{-h})\text{Id}\right),
\]
to obtain \((\bar{g}_0, \bar{v}_0) = (g_0, v^*)\);
(2) Solve the first-order Euler–Arnold equation, and approximate the Hamiltonian system using \(N\) leapfrog trajectories with step size \(\delta t > 0\). For example, for a matrix Lie groups with bi-invariant Riemannian metric, starting at \((\bar{g}_0, \bar{v}_0) = (g_0, v^*)\), we iterate [17]

\[
\text{For } k = 0, \ldots, N - 1:
\]
\[
\bar{v}_{k+1} = \bar{v}_k - \frac{\delta t}{2} \text{Tr}\left(\partial_x V^T \bar{g}_k \xi_k\right) \xi_k
\]
\[
\bar{g}_{k+1} = \bar{g}_k \exp\left(\delta t \bar{v}_{k+1}\right)
\]
\[
\bar{v}_{k+1} = \bar{v}_{k+1} - \frac{\delta t}{2} \text{Tr}\left(\partial_x V^T \bar{g}_{k+1} \xi_{k+1}\right) \xi_{k+1}
\]
to obtain \((\bar{g}_N, \bar{v}_N)\).
(3) Accept or reject the proposal by a Metropolis-Hastings step (although we note that implementing more advanced correction steps that take into account the whole trajectory is desirable [24]). We accept the proposal \((\bar{g}_N, \bar{v}_N)\) with probability
\[
\alpha = \min\{1, \exp(-H(\bar{g}_N, \bar{v}_N) + H(\bar{g}_0, \bar{v}_0))\}
\]
and set \((g_1, v_1) = (\bar{g}_N, \bar{v}_N)\). On the other hand, if the proposal is rejected, we set \((g_1, v_1) = (\bar{g}_0, -\bar{v}_0)\).

Compared to the algorithm presented in [17], our choice of noise field \(Y_i \equiv \partial_{\xi_i}\) as opposed to \(Y_i \equiv X_{U,\sigma}\) avoids having to compute matrix exponentials in the first step of the algorithm (which appears in the latter situation in the form \(e^{-\frac{1}{2}Dh}\), where \(D\) is a matrix given by \(D^j_i = Y_i^k Y^*_k\)), thus significantly reducing the computational cost. On the other hand, choosing noise fields of the form \(Y_i = X_{U,\sigma}\) may be useful when the potential energies \(U_i\) are adapted to the target distribution, for example by increasing the contribution of the noise at appropriate locations.

10. ERGODICITY OF \(\mathcal{A}\)-DIFFUSIONS

Ergodicity plays an important role in many of the applications in which measure-preserving diffusions are employed, so here we discuss the conditions that the drift and diffusion vector fields \((X, Y_i)\) must satisfy in order to ensure unique ergodicity of the diffusion \(dZ_t = X dt + Y_i \circ dW^i_t\). This will also allow us to clarify the conditions necessary for ergodicity in the Euclidean recipe [11].

First, let us denote by \(Z^\tau_t\) the solution to the SDE \(dZ_t = X dt + Y_i \circ dW^i_t\) with initial condition \(Z_0 = x\). In general, it is well-known that if the diffusion satifies:

(i) the strong Feller property, that is if the Markov semigroup \(T_t\) associated with the process \(Z^\tau_t\) maps all bounded measurable functions into continuous functions, and

---

6For a non-matrix group, simply replace \(\text{Tr}\left(\partial_x V^T \bar{g}_k \xi_k\right)\) with \(e_{\xi} V(V)\) [14].

7The Markov semigroup is defined as \(T_t f(x) = \int_M f(y)P_t(x, dy)\), where \(P_t(x, A) = \mathbb{P}(Z^\tau_t \in A)\) for all \(A \in \mathcal{B}(M)\).
Thus, contrary to the claim made in the Euclidean recipe [121, Theorem 1], it is not sufficient that $S(\alpha, \alpha) > C\|\alpha\|^2$ for any covector $\alpha \in T^*_x \mathbb{R}^n$, where $S = Y_t \otimes Y_t$. In particular, on compact manifolds $M$, it is sufficient that the diffusion is non-degenerate, meaning that its generator is only elliptic (see [27]). When the generator (21) is strongly elliptic, that is, the Lie algebra generated by $(Y_t)$ spans the tangent spaces $T_x M$ at every $x \in M$, then whenever a stationary measure exists, it must be unique on any paracompact, connected and orientable manifold $M$, as shown in [89, Proposition 6.1]. In particular, on compact manifolds $M$, it is sufficient that the diffusion is non-degenerate, meaning that its generator is only elliptic (see [27]). In Euclidean space, strong ellipticity means that there exist $C > 0$ such that $S(\alpha, \alpha) > C\|\alpha\|^2$ for any covector $\alpha \in T^*_x \mathbb{R}^n$, where $S = Y_t \otimes Y_t$. Thus, contrary to the claim made in the Euclidean recipe [121, Theorem 1], it is not sufficient that $S$ is positive definite (i.e., that the generator is elliptic) to ensure uniqueness of the target measure [89].

Unfortunately, many diffusions of interest are not elliptic (for example those with vertical noise), so it would be interesting to check in future works what precise conditions on $\mathcal{A}$ and $Y_i$ are required for Hörmander condition to hold in our $\mathcal{A}$-diffusion [29], given that $X = \{ Y_t \} \cup \{ \frac{1}{2} \text{curl}_P(Y_i) Y_i \}$. In particular, the subclass of Langevin-like volume-free processes studied in [30] is entirely made of rotationnals:

$$dZ_t = \left( X^\text{curl}_M(Y) - \frac{1}{2} \beta X^\text{curl}_M(\mathcal{A}) \otimes \text{curl}_M(\mathcal{A}) \right) dt + Y_t \circ dW^t$$

This insight may be useful in tackling the ergodicity problem in the non-elliptic case, especially when combined with the fact curl$_P$ has natural properties with respect to Lie brackets since it is a derivation of the Schouten–Nijenhuis bracket, a multi-vector generalisation of the Lie bracket [98].

We should also note that the dynamical ergodicity of the underlying stochastic process is not sufficient for building algorithms that are robust enough for practical use – it only provides an asymptotic guarantee for the behaviour of empirical averages of exact realizations of the stochastic process. The condition says nothing about the non-asymptotic behaviour of exact realizations nor any behaviour of the numerical discretizations to which we are limited to in practice. For example, MALA is obtained by applying an explicit Euler-Maruyama scheme to the overdamped Langevin process [29], and composing it with an accept-reject step. However, it is well-known that the algorithm does not maintain the ergodicity properties of the continuous process that it is derived from (see [147] for example).

To guarantee that the algorithm will be useful in practice, we need to bound the convergence of the discretized stochastic process towards its asymptotic limit, if one exists. Recent progress has been made in understanding the converge of both exact and discretized Langevin diffusions in Wasserstein distances [14, 94, 148, 56], although these results are limited to sufficiently nice target distributions that limit their practical utility.
Classic statistical results do not consider the convergence of diffusions themselves, but rather the Metropolis-Hastings transitions that use the discretized diffusions as a proposal distribution. Using coupling techniques, they demonstrate when the convergence admits geometric bounds in the total variation distance. Although these bounds are not particularly tight, they ensure the existence of central limit theorems which then allow for the convergence to be estimated well empirically.

When moving beyond diffusions to more general second-order Markov processes the problem becomes even harder. The limited theoretical results \cite{55,118} focus largely on necessary conditions for geometric bounds in the total variation distance and hence the existence of central limit theorems. Although these conditions are not sufficient to guarantee any particular non-asymptotic behavior, they motivate empirical diagnostics that help practitioners identify target distributions beyond the scope of the algorithm.

11. A Brief History of Measure-Preserving Diffusions

The history of measure-preserving processes is a long one, and in this section, we only aim to provide a handful of previous works that are directly related to this one. While in the machine learning community, the characterisation of measure-preserving diffusions on $\mathbb{R}^n$ was popularised in the recent NeurIPS article \cite{121}, anterior closely related results can be found in the SDE literature. For example in 1977, Robert Graham discusses the covariance of the Fokker–Planck equation, in the context of non-degenerate diffusions, and uses the Riemannian metric associated to the noise to define a Riemannian divergence which allows him to differentiate second-order tensors \cite{73} (a nice discussion of the work of Graham is also provided in \cite{60}). By analogy with Maxwell’s equations, Graham notes that the Fokker–Planck current must be the Riemannian divergence of some anti-symmetric tensor field, which is precisely the result provided in \cite{121,Theorem 2}. The covariance of the Fokker–Planck equation and the diffusion process is also discussed in \cite{19} and \cite{128}, where the latter article derives conditions for the diffusion to be reversible (see also \cite{134}). A less intuitive characterisation of the Fokker–Planck current of measure-preserving diffusions is also given in \cite{57} and in the case of non-degenerate diffusions on compact oriented manifolds, the book \cite{90} effectively derives a complete recipe using the Riemannian metric derived from the noise to transform the Fokker–Planck vector field into a 1-form, that is then studied via its Hodge–de Rham decomposition.

A major shortcoming of these references is that they all assume the noise to be non-degenerate, in order to equip the manifold with a Riemannian metric, as well as the orientability of the manifold to work with differential forms. Yet, many important measure-preserving diffusions are degenerate, such as (the deterministic) Hamiltonian systems, or even the underdamped Langevin process. While on Euclidean space, we have a “natural” metric that we can use to differentiate second-order tensors, such metrics do not exist on general manifolds. Concurrently to this article, a covariant formulation was introduced in \cite{48} to remove the dependence on the metric. However contrary to our recipe, this work relies on local coordinates, and does not take into account the presence of topological obstruction, thus leading to a recipe which is only valid locally, since on manifolds, there are divergence-free vector fields that cannot be globally expressed as the $P$-rotationnel of a bi-vector field. Moreover, the relation with the canonical geometry of $P$ is
not shown, and as we have illustrated in [86] our geometric framework offers new insights even on Euclidean space. More importantly, the intrinsic geometry of $P$ allows us to re-contextualise the theory of measure-preserving diffusion within the realm of differential geometry.

In the bigger picture, we see that these results are a combination of two things: the construction of the Fokker–Planck equation [62, 141, 97, 146] and its expression in geometric form as discussed above (see also [137]), combined with geometric characterisations of divergence-free vector field. Such characterisations have already been studied in several works on geometric integrators [130, 77] and have been known for at least a century, as seen in the work [45]. For example, the fact that vector fields that preserve the Lebesgue measure can be written as the divergence of an antisymmetric matrix (without any integrability assumption), which is all that is needed to obtain [121, Theorem. 2], goes back at least to the works of Poincaré and Volterra in the 1880s, e.g. [157].

12. Conclusion

In this work, building on from results in Poisson mechanics, geometry, topology, physics, and statistics, we have presented the complete and canonical characterisation of measure-preserving diffusions on arbitrary manifolds, which play a central role in many areas of science, both in terms of mathematical modelling and in statistics/machine learning. Our general framework provides a sound mathematical basis to design and study them. It not only extends and contextualise the results obtained in [121] for the Euclidean case, and improves it by removing the integrability constraint, but more importantly provides an elegant interpretation from a purely topological standpoint, relying solely on the geometry of the volume manifold $(M, P)$. This is achieved by constructing potentials for the Fokker-Planck current in the same way as how physical ‘potentials’ such as the potential energy and the magnetic potentials are constructed in classical mechanics. On contractible sample spaces, the resulting diffusion is specified, just as with thermodynamic systems, by two ‘brackets’: an antisymmetric $A$ that presents itself as the ‘potential’ for the Fokker-Planck current, and a dissipative one $S$, that is generated by the noise vector fields $(Y_i)$. Moreover, when the topology of the manifold is non-trivial (e.g., it is not connected), we also need to take into account an extra topological obstruction term to achieve global completeness, which we have shown to be parametrised by harmonic forms on compact orientable manifolds, and non-zero elements of a twisted de Rham cohomology group in general.

In addition to fully characterising the measure-preserving diffusions, we have also studied their reversibility, associated flows on the space of volume measures, the generalisations of Langevin processes to manifolds, and introduced a new recipe for volume-free diffusions that are well-suited to the construction of Langevin-like sampling algorithms. Our canonical formulation properly takes into account the critical assumptions on the target measure, namely, that it is smooth and globally supported, which allows us to analyse the diffusions through measure-informed versions of known results in differential geometry (obtained using isomorphisms induced by the target). From a practical point of view, having intrinsic results that focus on the target measure and do not make any extra assumptions imply that these can be applied regardless of the particular application, such as physics and machine learning. In future works, we will further address how to develop efficient
MCMC algorithms to sample from manifolds using this complete recipe, and furthermore, we aim to extend this framework in the context of infinite-dimensional diffusions, as considered in [22, 100, 139], which may be useful for applications in stochastic climate modelling and data assimilation [31, 64, 99, 122, 123, 124].

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Appendix A. Proofs

A.1. Derivation of Fokker–Planck operator.

**Lemma A.1.** Given smooth vector fields $X, Y_1, \ldots, Y_N$ on $M$, consider the Stratonovich SDE

$$dZ_t = X(Z_t) \, dt + Y_i(Z_t) \circ dW^i_t.$$  

Then its generator is given by $L f = X f + \frac{1}{2} \sum_i Y_i Y_i f$. The Fokker–Planck operator, viewed as the formal adjoint of $L$ in $L^2(\mu_M)$ (if the boundary $\partial M$ is non-empty we restrict to functions that vanish on the boundary) is given by

$$L^* f = \text{div} \mu_M \left( -f X + \frac{1}{2} \sum_i Y_i Y_i f \right).$$

**Proof.** Vector fields satisfy Leibniz rule

$$\int g X(f) \mu_M = \int X(gf) \mu_M - \int f X(g) \mu_M,$$

and note that $\int_M \text{div}(X) \mu_M = \int_M i_X \mu_M = \int_{\partial M} g i_X \mu_M$ which vanishes if $g|_{\partial M} = 0$ (here div $\equiv \text{div}_{\mu_M}$). Hence

$$\int g X(f) \mu_M = - \int g \text{div}(X) \mu_M - \int f X(g) \mu_M$$

$$= \int f (-g \text{div}(X) - X(g)) \mu_M$$

$$= \int f (-\text{div}(g X)) \mu_M = \int f L^* g \mu_M.$$ 

Now let us compute the adjoint of the diffusion component. First note that

$$Y_k(g Y_k f) = \text{div}(g Y_k f Y_k) - g Y_k f \text{div}(Y_k) =$$

$$= \text{div}(g Y_k f Y_k) - f \text{div}(g Y_k Y_k) + f \text{div}(g \text{div}(Y_k) Y_k)$$

and

$$Y_i g Y_i f = \text{div}(f Y_i g Y_i) - f \text{div}(Y_i g Y_i).$$

It follows that if $f, g$ vanish on the boundary

$$\frac{1}{2} \int g Y_i Y_i f \mu_M = \frac{1}{2} \int (Y_i(g Y_i f) - Y_i g Y_i f) \mu_M$$

$$= \frac{1}{2} \int \left( f \text{div}(g Y_i Y_i) + f \text{div}(Y_i g Y_i) \right) \mu_M$$

$$= \int f \frac{1}{2} \text{div}(g Y_i Y_i) \mu_M = \int f L^* g \mu_M.$$

A.2. Proof of Theorem 2.4

**Theorem A.2.** The Gibbs measure (4) is preserved under the bracket diffusion (7), in the sense that $L^* p_\infty = 0$, if and only if the vector field $Y$ satisfies

$$(42) \quad \text{div}_{\mu_M}(X_{p_\infty} - \beta_{p_\infty} Y) = 0.$$
Proof. Let \( p(x) = \frac{1}{\sqrt{2\pi}} e^{-\beta x} \) for \( x \in \mathbb{R} \), so \( p_\infty = p \circ H : \mathbb{M} \to \mathbb{R} \), and \( X_{p_\infty} = -p_\infty X_H \).

Then using the Fokker-Planck operator defined in (6), we have
\[
\mathcal{L}^* p_\infty = \text{div} \left( -p_\infty \left( X_H - \frac{\beta}{2} Y_i(H)Y_i + \frac{1}{2} \text{div}(Y_i)Y_i + Y \right) + \frac{1}{2} \text{div}(p_\infty)Y_i \right)
\]
\[
= \text{div} \left( \frac{1}{\beta} X_{p_\infty} - p_\infty Y - \frac{1}{2} Y_i(p_\infty)Y_i - \frac{1}{2} \text{div}(Y_i)Y_i + \frac{1}{2} \text{div}(p_\infty)Y_i \right)
\]
\[
= \text{div} \left( \frac{1}{\beta} X_{p_\infty} - p_\infty Y - \frac{1}{2} \text{div}(p_\infty)Y_iY_i + \frac{1}{2} \text{div}(p_\infty)Y_i \right)
\]
\[
= \text{div} \left( \frac{1}{\beta} X_{p_\infty} - p_\infty Y \right),
\]

thus \( \mathcal{L}^* p_\infty = 0 \) iff \( Y \) satisfies \( \text{div} \left( \frac{1}{\beta} X_{p_\infty} - p_\infty Y \right) = 0. \)

A.3. Recovering The Euclidean Complete Recipe.

Corollary A.3. Let \( \mathcal{M} = \mathbb{R}^n \) with flat metric, \( \mu_\mathcal{M} = dx \), \( \sigma_{ij} \equiv Y^j_i \), \( D \equiv \frac{1}{\beta} \sigma \sigma^T \) and \( Q_{ij} \equiv \mathcal{A}^{ij} \). Then (7) reduces to the Itô diffusion considered in the complete recipe for SGMCMC [121]
\[
\frac{dZ_t}{\sqrt{Q}} = -(Q + D) \nabla H dt + \nabla \cdot (Q + D) dt + \sqrt{2D} dw_t,
\]
where we use the convention \( \langle \nabla \cdot Q \rangle_i \equiv \partial_j Q_{ij} \) as in [121].

Proof. In that case, the term \( Y_i(H)Y_i = Y^j_iY^k_i \partial_jH \partial_k \) represents the "symmetric semi-definite part" of the dynamics since in flat space this is \( (\sigma \sigma^T)_{jk} \partial_jH \partial_k \) where \( \sigma_{ij} = \sigma^j_i = Y^j_i \), while the term \( \text{div}(Y_i)Y_i = \sigma_{ki} \partial_j \sigma_{ji} \partial_k \) together with the Itô-to-Stdatonovich correction yields the divergence of the diffusion matrix \( D \equiv \frac{1}{\beta} \sigma \sigma^T \).

Using the convention \( \langle \nabla \cdot Q \rangle_i \equiv \partial_j Q_{ij} \) in [121]
\[
\frac{dZ_t}{\sqrt{Q}} = \left( \mathcal{A}^{ij} \partial_j H \partial_i - \frac{\beta}{2} (\sigma \sigma^T)_{jk} \partial_j H \partial_k \right) dt
\]
\[
+ \sigma_{ij} \partial_i \circ dW^j_t
\]
\[
\left( \mathcal{A}^{ij} \partial_j H \partial_i - \frac{\beta}{2} (\sigma \sigma^T)_{jk} \partial_j H \partial_k + \frac{1}{2} \sigma_{ki} \partial_j \sigma_{ji} \partial_k + \frac{1}{2} \sigma_{ki} \partial_k \sigma_{ji} \partial_j + \partial_j \mathcal{A}^{ij} \partial_i \right) dt
\]
\[
+ \sigma_{ij} \partial_i dW^j_t
\]
\[
= (-Q \nabla H - \beta D \nabla H + \nabla \cdot D + \nabla \cdot Q) dt + \sqrt{2D} dw_t.
\]

A.4. Derivation that Curl is Modular Field. This result was proved in the thesis of one of the authors [14], but the proof relies on introducing Schouten-Nijenhuis brackets. Thus we here include a new direct and more constructive proof:

Proof. We will prove the equivalence by demonstrating that the action of the modular vector field and the curl vector field are equal for all smooth functions \( f \),
\[
\text{curl}_P(\mathcal{A})(f) \cdot P = X^P_\mathcal{A}(f) \cdot P.
\]
The curl vector field is defined implicitly by the action
\[ i_{\text{curl}(A)}P = d\left(P^b(A)\right) \]
which implies that for any \( f \)
\[ df \wedge i_{\text{curl}(A)}P = df \wedge d\left(P^b(A)\right). \] (44)
To simplify the left hand side note that
\[ 0 = i_{\text{curl}(A)}(df \wedge P) = i_{\text{curl}(A)}(df) \cdot P - df \wedge i_{\text{curl}(A)}P = \text{curl}(A)(f) \cdot P - df \wedge i_{\text{curl}(A)}P, \]
or
\[ df \wedge i_{\text{curl}(A)}P = \text{curl}(A)(f) \cdot P. \]
For the right hand side we take
\[ d\left(df \wedge (P^b(A))\right) = d^2f \wedge P^b(A) - df \wedge d\left(P^b(A)\right) = -df \wedge d\left(P^b(A)\right). \]
Substituting both results in Equation (44) then gives
\[ \text{curl}(A)(f) \cdot P = -d\left(df \wedge P^b(A)\right). \] (45)
Now we use the fact that for any function \( P^b(df \wedge P^b(A)) = i_{df}A \) [2], so that equation (45) becomes
\[ \text{curl}(A)(f) \cdot P = -dP^b(i_{df}A) = dP^b\left(X_f^A\right) = \text{div}_P(X_f^A) \cdot P \]
as desired.
□

A.5. Derivation of Adjoint of Integration Pairing.

**Lemma A.4.** The Fokker–Planck operator of the Stratonovich SDE [3], viewed as the formal adjoint of \( \mathcal{L} \) with respect to the pairing \( \langle f, P \rangle \mapsto \int f dP \) between smooth, compactly supported functions \( f \) and smooth measures \( P \), is given by
\[ \mathcal{L}^*P = -\mathcal{L}_X P + \frac{1}{2} \mathcal{L}_{Y_i} \mathcal{L}_{Y_i} P. \] (46)

**Proof.** Recall the generator is \( \mathcal{L} = X + 4Y_i \circ Y_i \). Thus for the deterministic drift we find
\[ \int X(f)P = \int df(X)P = \int i_X(df)P = \int df \wedge i_XP = \int df \wedge i_XP = \int fL_XP. \]
Similarly, for the diffusion coefficient,
\[ \int Y_iY_i(f)P = -\int Y_i(f)\mathcal{L}_{Y_i}P = \int f\mathcal{L}_{Y_i} \mathcal{L}_{Y_i}P. \]
□
A.6. Derivation of $\mathcal{A}$-diffusion expressed in terms of the reference measure $\mu_M$. Here, we include additional details to the derivation of the $\mathcal{A}$-diffusion in terms of reference measure $\mu_M$ from the abstract $\mathcal{A}$-diffusion [11].

In terms of the target $P = e^{-\beta H} \mu_M$. First note that if $f$ is a non-vanishing function, then $(f \mu_M)^\flat = f \mu_M^\flat$ and so $(f \mu_M)^\sharp = \mu_M^\sharp \circ \frac{1}{f}$. Hence
\begin{align*}
\operatorname{curl}_{f \mu_M}(X) &= (f \mu_M)^\sharp \circ \mathbf{d} \circ (f \mu_M)^\flat(Y)(X) = (\mu_M)^\flat \left( \frac{1}{f} \mathbf{d} \left( f (\mu_M)^\flat(Y)(X) \right) \right) \\
&= (\mu_M)^\sharp \circ \mathbf{d} \circ (\mu_M)^\flat(Y)(X) + (\mu_M)^\sharp \left( \frac{1}{f} \mathbf{d}f \right) \wedge (\mu_M)^\flat(Y)(X)
\end{align*}
where $\mathbf{d}f \equiv \mathbf{d} \log |f|$ is the distorted de Rham derivative.

**Proposition A.5.** Given $P = e^{-\beta H} \mu_M$, we have
\begin{align}
\frac{\partial Y}{\partial t} &= \frac{1}{2} \mathbf{R}(Y) - \beta Y(H), \\
\operatorname{curl}_P(\mathcal{A}) &= X^\mu_M + \beta X^\mathcal{A}_H,
\end{align}
for any vector field $Y \in \mathfrak{X}(\mathcal{M})$ and bi-vector field $\mathcal{A} \in \mathfrak{X}^2(\mathcal{M})$.

**Proof.** Taking $f = e^{-\beta H}$ in the above, we have
\begin{align*}
\operatorname{div}_P(Y) &= \operatorname{curl}_P(Y) = (\mu_M)^\sharp \circ \mathbf{d} \circ (\mu_M)^\flat(Y) - \beta (\mu_M)^\flat \left( \mathbf{d}H \wedge (\mu_M)^\flat(Y) \right) \\
&= \operatorname{div}_{\mu_M}(Y) - \beta (\mu_M)^\flat \left( \mathbf{d}H \wedge (\mu_M)^\flat(Y) \right).
\end{align*}
Now, using the identity $i_Y(\mathbf{d}H \wedge \mu_M) = i_Y \mathbf{d}H \wedge \mu_M = \mathbf{d}H \wedge i_Y \mu_M$ and noting that $\mathbf{d}H \wedge \mu_M = 0$ (since $\mu_M$ is a top degree twisted form on $\mathcal{M}$), we have $\mathbf{d}H \wedge i_Y \mu_M = i_Y \mathbf{d}H \wedge \mu_M = (\mu_M)^\flat(Y(H))$. The first identity (47) then follows immediately.

Similarly, we have
\begin{align*}
\operatorname{curl}_P(\mathcal{A}) &= \operatorname{curl}_{\mu_M}(\mathcal{A}) - \beta (\mu_M)^\flat \left( \mathbf{d}H \wedge (\mu_M)^\flat(\mathcal{A}) \right).
\end{align*}
Noting that $(\mu_M)^\flat(\mathbf{d}H \wedge (\mu_M)^\flat(\mathcal{A})) = i_{\mathbf{d}H} \mathcal{A} \equiv -X^\mathcal{A}_H$ (see [12]) and $\operatorname{curl}_{\mu_M}(\mathcal{A}) = X^\mu_M$ (see [13], the second identity (48) follows.

A.7. Derivation of Measure-Preserving Diffusion on Riemannian Manifolds.

**Theorem A.6.** Let $\mathcal{M}$ be a compact orientable Riemannian manifold and let $\mu_M \equiv \operatorname{vol}$ and $\nabla \cdot$ denote respectively the Riemannian measure and divergence. Then, any $e^{-H}$ vol-preserving diffusion has the form
\begin{align}
\frac{\partial g}{\partial t} &= \mathcal{L}^* g = \delta \left( -gX + \frac{1}{2} \nabla \cdot (gY_1)Y_1 \right),
\end{align}
where $\star$ is the Hodge star operator, $\sharp$ is the Riemannian musical isomorphism, $\mathcal{A}$ is an antisymmetric bracket and $\zeta$ is a harmonic $(n-1)$-form (i.e., it satisfies “Maxwell’s equations” $d\zeta = 0$, $d \star \zeta = 0$).

**Proof.** Let $\delta \propto \star \mathbf{d} \star$ be the co-differential. Since $\operatorname{div}_{\operatorname{vol}} = \delta \circ \flat$, the Fokker-Planck operator [10] may be written as
\begin{align}
\mathcal{L}^* g &= \delta \left( -gX + \frac{1}{2} \nabla \cdot (gY_1)Y_1 \right).
\end{align}
It then follows by the Hodge decomposition that $L^* p_\infty = 0$ iff $\delta ( - p_\infty X + \frac{1}{2} \nabla \cdot (p_\infty Y_i) Y_i )^b = 0$ iff $d \star (- p_\infty X + \frac{1}{2} \nabla \cdot (p_\infty Y_i) Y_i )^b = 0$ iff $\gamma$ is Harmonic, that is co-exact and closed, and vanishes whenever the $\dim(M) - 1$ de Rham cohomology is trivial. Thus $(- p_\infty X + \frac{1}{2} \nabla \cdot (p_\infty Y_i) Y_i )^b = \delta \varepsilon - \ast^{-1} \gamma$ where $\varepsilon \equiv \ast^{-1} \alpha$ is a 2-form. Hence,

$$- p_\infty X + \frac{1}{2} \nabla \cdot (p_\infty Y_i) Y_i = \frac{1}{2} \delta \varepsilon + \frac{1}{2} \ast^{-1} \gamma = \nabla \cdot (A p_\infty) - \frac{1}{2} \ast^{-1} \gamma,$$

for an appropriate antisymmetric bracket $A$. Now, $\nabla \cdot (A p_\infty) = p_\infty \nabla \cdot A - p_\infty X_H$, since $\nabla \cdot A = \text{curl}_{\text{vol}}(A)$ (proved below), and for any $f$

$$\text{curl}_\mu(p_\infty A)[f] = - \text{div}_\mu(p_\infty X_f) = - X_f(p_\infty) - p_\infty \text{div}_\mu X_f = + p_\infty X_f(H) - p_\infty \text{div}_\mu X_f$$

$$= - p_\infty X_H(f) - p_\infty \text{div}_\mu X_f,$$

so

$$\text{curl}_\mu(p_\infty A) = - p_\infty X_H + p_\infty \text{curl}_\mu A.$$

It follows that the drift vector field must take the form

$$X = X_H + \frac{1}{2} \nabla \cdot (Y_i) Y_i - \frac{1}{2} Y_i(H) Y_i - \nabla \cdot A + e^H \frac{1}{2} \ast^{-1} \gamma.$$

Note that the Riemann divergence $\nabla \cdot A$ in the previous theorem is precisely the curl of the Riemann measure (up to a sign). Indeed, if $(M, M)$ is a pseudo-Riemannian manifold, recall that $\nabla \cdot A = \text{Tr} \nabla A$, where $\text{Tr}$ is the trace and $\nabla$ the covariant derivative. Then using the fact that $S_{ab} A^{ab} = 0$ for any symmetric tensor $S_{ab}$ and anti-symmetric tensor $A^{ab}$, we see that for any smooth function $f$

$$\nabla \cdot (f \nabla \cdot A) = \frac{1}{|M|} \partial_a \left( f \partial_a (\sqrt{|M| A^{ab}}) \right) = \frac{1}{|M|} (\partial_a f) \left( \partial_a (\sqrt{|M| A^{ab}}) \right)$$

$$= \frac{1}{|M|} \partial_a \left( \sqrt{|M| A^{ab}} \partial_b f \right) = \frac{1}{|M|} \partial_a \left( \sqrt{|M| X_f^a} \right) = - \nabla \cdot X_f^a,$$

so from (3) applied to $\mu_M = \text{vol}$ and $f = p_\infty$, we see that $\nabla \cdot A = - X_{\text{vol}}^a = - \text{curl}_{\text{vol}}(A)$.

A.8. Derivations for the Reversibility Section. Recall that $X_{\mathcal{B}}^p(f) \equiv \text{div}_P(X_{\mathcal{B}}^p)$ for any bracket $\mathcal{B}$. Then

**Corollary A.7.** The generator of a $P$-preserving expressed in the form of (2) can be written as

$$L f = X_{\mathcal{B}}^p(f) + P^q(\gamma)(f) + \frac{1}{2} X_{\mathcal{A}}^p(f).$$

Moreover, $\mathcal{B} X_{\mathcal{B}}^p$ is symmetric in $L^2(P)$, while $X_{\mathcal{A}}^p$ and $P^q(\gamma)$ are both antisymmetric in $L^2(P)$,

$$\langle X_{\mathcal{A}}^p f, h \rangle_P = - \langle f, X_{\mathcal{A}}^p h \rangle_P, \quad \langle X_{\mathcal{B}}^p f, h \rangle_P = \langle f, X_{\mathcal{B}}^p h \rangle_P,$$

where $\langle \cdot, \cdot \rangle_P$ denotes the $L^2(P)$ pseudo-inner product, $\langle f, h \rangle_P \equiv \int f h \, dP$. Hence, $L$ is symmetric if and only if $X_{\mathcal{A}}^p + P^q(\gamma) = 0$. In general, the generator of (4) satisfies $L = \mathcal{B} X_{\mathcal{B}}^p$ if and only if the Fokker-Planck current of $P$ vanishes, in which
case, we say that \( \mathcal{L} \) satisfies the detailed balance condition, and the diffusion is reversible. Finally, \( \mathcal{L} X^P_S \) is non-positive, i.e.,

\[
\langle \mathcal{L} X^P_S(f), f \rangle_p \leq 0
\]

for all \( f \in C^\infty_c(M) \).

**Proof.** The formula for the generator follows from \([19]\) and \( \text{div}_P(X^P_Y) = \text{div}_P(Y_i)Y_i(f) + Y_iY_i(f) \), as we prove using a local argument: given local coordinates \((z^i)\), writing \( P = p_\infty dz \) we have

\[
\text{div}_P(X^P_Y) = \frac{1}{p_\infty} \partial_t(p_\infty S^\nu \partial_j f) = \frac{1}{p_\infty} \partial_t(p_\infty Y_i^j \partial_j f) = \text{div}_P(Y_i)Y_i(f) + \partial_t(Y_i^j \partial_j f)Y_i^r,
\]

which, combined with the fact that for any vector field \( Y \), \( YY(f) = Y^i \partial_i (Y^j \partial_j f) = Y^i \partial_i Y^j \partial_j f + Y^i \partial_i Y^j \partial_j f \), yields the result. From the proof of proposition \([A.1]\) we know the (formal) adjoint of \( X^P_A \) is \( f \mapsto -\text{div}_P(f X^P_A) \), and \(-\text{div}_P(f X^P_A) = -X^P_A(f) - f \text{div}_P(X^P_A) = -X^P_A(f) \). Indeed, this only requires the fact that the dynamics \( X^P_A \) preserves \( P \), and thus still holds when we include the topological obstruction contribution, which has itself vanishing \( \text{div}_P \). From \([6]\) we also know that the adjoint of \( X^P_P \) is \( f \mapsto -\text{div}_P(f \text{div}_P(Y_i)Y_i) + \text{div}_P(\text{div}_P(fY_i)Y_i) = \text{div}_P(Y_i(f)Y_i) = \text{div}_P(X^P_P) = X^P_P(f) \).

We denote the pushforward with respect to a diffeomorphism \( \mathcal{R} \) on tensor fields by \( \mathcal{R}_* \). Then

**Corollary A.8.** Let \( \mathcal{R} \) be a target-preserving diffeomorphism, which is an \( \mathcal{A} \)-antimorphism and a \( \mathcal{S} \)-morphism, that is

\[
\mathcal{R}_* \mathcal{A} = -\mathcal{A}, \quad \mathcal{R}_* \mathcal{S} = \mathcal{S}.
\]

Then, the generator of the \( \mathcal{A} \)-diffusion \([21]\) is reversible up to \( \mathcal{R} \), that is we have

\[
\langle f, \mathcal{L} h \rangle_p = \langle \mathcal{L} \mathcal{R}^* f, \mathcal{R}^* h \rangle_p, \quad \forall f, h \in C^\infty_c(M).
\]

**Proof.** First note that for any \( \mathcal{B} \)-Hamiltonian vector field, since \( \mathcal{R}^* P = P \), then, using proposition 6.3.5 \([2]\), \( \mathcal{R}^* \mathcal{L}_{X^P} \mathcal{R}^* P = \mathcal{L}_{(\mathcal{R}^{-1})_* X^P} \mathcal{R}^* P = \mathcal{L}_{(\mathcal{R}^{-1})_* X^P} P \), so \( \text{div}_P((X^P) \circ \mathcal{R} = \text{div}_P((\mathcal{R}^{-1})_* X^P) \). Now consider the antisymmetric part, \( \mathcal{L} = X^P_A \). Then \( \langle f, X^P_A h \rangle_p = -\langle X^P_A f, h \rangle_p = -\langle \mathcal{R}^* X^P_A f, \mathcal{R}^* h \rangle_p \), where we have used \( \mathcal{R}_* P = P \) in the last equality. Moreover \( \mathcal{R}^* X^P_A f = -X^P_A \mathcal{R}^* f \) since \( \mathcal{R} \) is an \( \mathcal{A} \)-antimorphism, \( (\mathcal{R}^{-1})_* X^P_A = -X^P_A \mathcal{R} \). The proof of the symmetric part is analogous, except we have \( \mathcal{R}^* X^S_P f = X^S_P \mathcal{R}^* f \). Note that if \( \mathcal{R}_* Y_i = \pm Y_i \) then \( \mathcal{R} \) is a \( \mathcal{S} \)-morphism, since \( (\mathcal{R}^{-1})_* X^S_P (\mathcal{R}^* Y_i(f)) Y_i = Y_i(f) \circ \mathcal{R}(\mathcal{R}^{-1})_* Y_i = (\mathcal{R}_* (\mathcal{R}^{-1})_* Y_i)(f) \circ \mathcal{R}(\mathcal{R}^{-1})_* Y_i = (\mathcal{R}_* Y_i)(\mathcal{R}^* f)(\mathcal{R}^{-1})_* Y_i = Y_i(\mathcal{R}^* f) Y_i = X^S_{\mathcal{R}^{-1}_*} f \).

**A.9. Non-Degenerate and Overdamped Systems.**

**Theorem A.9.** Any \( P \propto p_\infty \log P \) diffusion generated by \([27]\) takes, at least up to topological obstructions, the form \([25]\) for some \( \mathcal{A} \in \mathfrak{X}^2(M) \) (\( \nabla \) is the Riemannian gradient)

\[
dZ_t = \frac{1}{2} \nabla \log p_\infty(Z_t)dt - X^A_{\log p_\infty}(Z_t)dt - \nabla \cdot \mathcal{A}(Z_t)dt + dB_t.
\]
Proof. Since $\Delta$ is symmetric in $L^2(M, \text{vol})$,$$
abla^*_{p_\infty} = -\nabla \cdot (p_\infty X) + \frac{1}{2} \Delta p_\infty = \nabla \cdot (-p_\infty X + \frac{1}{2} \nabla p_\infty),$$Thus, following the proof in §A.7$$-p_\infty X + \frac{1}{2} \nabla p_\infty = \nabla \cdot (A_{p_\infty}) = p_\infty \nabla \cdot A + p_\infty X_{{\log p_\infty}},$$at least locally (we refer to [90] for an analysis of non-degenerate measure-preserving diffusions in the case of compact oriented manifolds), and thus the drift has the form$$X = \frac{1}{2} \nabla \log p_\infty - \nabla \cdot A - X_{{\log p_\infty}},$$has claimed. $\square$

A.10. Rate of Change of Functionals along Measure-preserving Diffusions.

Proposition A.10. Let $F$ be a functional on the space of volume measures, and suppose $\frac{\delta F}{\delta \mu}$ is compactly supported, or more generally provided Stokes theorem holds. The rate of change of $F$ along the $P$-preserving diffusion is given by$$\frac{d}{dt} F(\mu_t) = \left\{ \log \frac{dP}{d\mu_t}, \frac{\delta F}{\delta \mu_t} \right\}_{\mathcal{T}}(\mu_t) + \left\{ \frac{d\mu_t}{dP}, \mu_t(\gamma) \right\}_{\mathcal{T}} \left( \frac{\delta F}{\delta \mu_t} \right),$$where $\mathcal{T}$ is the thermodynamic bracket $S/\sqrt{2} - A$, and $\gamma$ the topological obstruction.

Proof. Differentiating we have$$\frac{d}{dt} F(\mu_t) = \int \frac{\delta F}{\delta \mu_t} \frac{d\mu_t}{dt} = \int \frac{\delta F}{\delta \mu_t} \text{div}_{\mu_t} \left( X_{{\log \frac{dP}{d\mu_t}}} - \frac{1}{2} X_{{\log \frac{dP}{d\mu_t}}} \right) \mu_t.$$If $\frac{\delta F}{\delta \mu_t}$ is compactly supported, or more generally provided Stokes theorem holds, we have$$\frac{d}{dt} F(\mu_t) = -\int \left( X_{{\log \frac{dP}{d\mu_t}}} \left( \frac{\delta F}{\delta \mu_t} \right) - \frac{1}{2} X_{{\log \frac{dP}{d\mu_t}}} \left( \frac{\delta F}{\delta \mu_t} \right) \right) \mu_t.$$Hence$$\frac{d}{dt} F(\mu_t) = -\left\{ \log \frac{dP}{d\mu_t}, \frac{\delta F}{\delta \mu_t} \right\}_{\mathcal{T}}(\mu_t) + \frac{1}{2} \left\{ \log \frac{dP}{d\mu_t}, \frac{\delta F}{\delta \mu_t} \right\}_{\mathcal{T}}(\mu_t),$$which can be expressed as$$\frac{d}{dt} F(\mu_t) = \left\{ \log \frac{dP}{d\mu_t}, \frac{\delta F}{\delta \mu_t} \right\}_{\mathcal{T}}(\mu_t)$$via the thermodynamic bracket $\mathcal{T} = S/\sqrt{2} - A$ of the diffusion.

For the topological obstruction contribution, note that since $\mu_t(\gamma)$ is $\mu_t$ preserving,$$-\int \frac{\delta F}{\delta \mu_t} \mu_t(\gamma) \left( \frac{d\mu_t}{dP} \right) \mu_t = \int \mu_t(\gamma) \left( \frac{\delta F}{\delta \mu_t} \right) \frac{d\mu_t}{dP} \mu_t.$$Note that when $F \equiv \text{KL}(\cdot \| P)$ we have$$\frac{\delta \text{KL}(\cdot \| P)}{\delta \mu_t} = \log \frac{d\mu_t}{dP} = -\log \frac{dP}{d\mu_t},$$so we recover the formula for the rate of change of KL. $\square$
A.11. Underdamped Langevin on Manifolds.

**Theorem A.11.** Suppose \((\mathcal{A}, \mu_{TM})\) is a Langevin pair. If we choose the noise fields to be the vertical fields \(Y_i \equiv V \circ X_i \circ \pi\) for \(X_i \in \mathfrak{X}(M)\), then the \(\mathcal{A}\)-diffusion generated by \(e^{-H} \mu_{TM}\), with \(H \equiv \pi^* V + \frac{1}{2} \| \cdot \|^2\), is

\[
\text{d}(q_t, v_t) = \underbrace{X^\mathcal{A}_H(q_t, v_t) \text{d}t}_\text{\(\mathcal{A}\)-Hamiltonian dynamic} - \underbrace{\frac{\beta}{2} \langle X_i(q_t), v_t \rangle_{q_t} \text{d}t + V(X_i(q_t)) \text{d}W_t}_\text{vertical kinetic Dissipation} + \underbrace{\text{vertical randomness}}
\]

or in tangent-lifted coordinates

\[
\text{d}(q_t, v_t) = \left( X^\mathcal{A}_H(q_t, v_t) - \frac{\beta}{2} M(q_t) v_t \right) \text{d}t + \sigma(q_t) \circ \text{d}W_t,
\]

where \(M(q)v = M(q)_{\nu j} v^j \partial_{\nu} \equiv (\sigma^T M(q))_{\nu j} v^j \partial_{\nu}\) and \(\sigma \equiv \sigma_{j i} \partial_{\nu} = (X^j_i) \partial_{\nu}\), and \(\mathcal{M}_{j i}(q) = (\partial_{x^j}, \partial_{x^i})_q\). In particular \((\Pi, \omega^n_\mathcal{V})\) is a Langevin pair, where \(\Pi\) is the Poisson 2-vector field associated to \(\omega^n_\mathcal{V}\).

**Proof.** Recall the definition of the vertical lift \(V : v_q \mapsto \text{ver}_v v_q \in T\mathcal{F}\), with \(\text{ver}_v v_q : f \mapsto 4 \frac{\partial f(q, v_q + tv_q)}{\partial v_q}|_{t=0}\) for any \(f \in C^1(\mathcal{F})\). For example if \(\mathcal{F} = \mathbb{R}^n \times \mathbb{R}^l\) is a vector bundle of \(M = \mathbb{R}^n\), this is just the directional derivative of \(f\) at \((q, v_q)\) in the direction \((0, v_q)\), \((0, v) \cdot \nabla f(q, v) = v^k \partial_k f(q, v)\), or \(V = v^k \partial_k\), where \((x^a, v^j)\) are coordinates on \(\mathcal{F}\). If \(X \in \mathfrak{X}(M)\) is a vector field, with local expansion \(X = \Pi(X)(\partial_{x^i})\), then its composition with the canonical vector field \(\mathcal{V} \circ X \circ \pi \in \mathcal{X}(T\mathcal{F})\) is \(\mathcal{V} \circ X \circ \pi(x, v) = X^k(x) \partial_{x^i}\). Then if \(\mathcal{M}\) is a vector bundle Riemannian metric on \(\mathcal{F}\), and \(T\) is the associated kinetic energy we find

\[
Y_i(H)(x, v) = X^k_i(x) \partial_{x^i} (V(x) + T(x, v)) = X^k_i(x) \partial_{x^i} \left( \frac{1}{2} \mathcal{M}_{ji}(x) v^j v^j \right)
= X^k_i(x) \mathcal{M}_{ji}(x) v^j = \langle Y_i(x), v \rangle_x.
\]

Now consider \(\mathcal{F} = TM\). The above derivation shows we can also write

\[
Y_i(H)(x, v) = \langle X_i(x), v \rangle_x,
\]

from which \([31]\) follows. Moreover, setting \(\sigma_{ji} \equiv X^j_i\), so \(Y_i(x, v) = \sigma_{ji} \partial_{x^i}\) where \(v^j\) are the tangent-lifted coordinates \([3]\). We have

\[
Y_i(H)Y_i(x, v) = \langle X_i(x), v \rangle_x \text{ver}_{X_i(x)}(X_i(x)) = X^k_i(x) \mathcal{M}_{ji}(x) v^j X^l_i(x) \partial_{x^l}
= \sigma_{li}(x) \mathcal{M}_{ji}(x) v^j \sigma_{rj}(x) \partial_{x^r} = \left( \sigma^\top(x) \right)_{rk} \mathcal{M}_{ji}(x) v^j \partial_{x^r},
\]

and the local expression \([32]\) follows. Moreover the symplectic measure is indeed horizontal (this fact may be traced back to the fact that the Liouville 1-form is horizontal). Indeed, in tangent-lifted coordinates \(\omega^n_\mathcal{V} = |\mathcal{M}| \text{d}x^a \text{d}v^j\), so locally the divergence of \(Z \in \mathfrak{X}(TM)\) is \(\text{div}_{\omega^n_\mathcal{V}}(Z) = \frac{1}{|\mathcal{M}|} \partial_{x^a} (|\mathcal{M}| Z^a) + \partial_{v^j} Z^j\), and from the previous local expressions we see \(\text{div}_{\omega^n_\mathcal{V}}(Y_i) = 0\), and thus \(\omega^n_\mathcal{V}\) is horizontal.

Finally we mention that if the noise vector fields are chosen to be \(\Pi\)-Hamiltonian vector fields associated to “noise” Hamiltonians \(U_i : M \to \mathbb{R}\), then \(Y_i \equiv \mathcal{X}_U\|_{\text{ver}} = -\mathcal{V} \circ \nabla U_i \circ \pi\), i.e., they are the vertical lift of the Riemannian gradients, and \(Y_i(H) = \omega^n_\mathcal{V}(\mathcal{X}_H, \mathcal{X}_U\|_{\text{ver}}) = -\mathcal{X}_H(U_i \circ \pi) = -dU_i \circ \partial\pi(X^H_i) = -dU_i \circ \partial\pi(X^H_i)\) since \(X_V\) is vertical.

\(\square\)
Appendix B. Unpublished Result

The following results were proven in the thesis of one of the authors [14], and are being submitted as part of an article discussing the intrinsic geometry of smooth measures and its relations to various fields of mathematics. When this latter paper will be available online, this section will be erased and the mentions of it in the main article will be replaced by citations, but in the meantime, for completeness, we include the characterisation [15,1] of measure-preserving dynamical systems and its proof that we will use in the main article.

Denote by $\Omega^k(\mathcal{M})$ the space of twisted differential $k$-forms, that is differential $k$-forms taking value in the orientation bundle. In particular the smooth positive measure $P$ can be identified with a twisted form of top rank. For any $X \in \mathcal{X}^k(\mathcal{M})$, using $(\mathcal{X}^l(\mathcal{M}))^* \cong \Omega^l(\mathcal{M})$, we define the right interior product by $i_X P(A) \equiv \langle P, X \wedge A \rangle_*$ for any $A \in \mathcal{X}^{n-k}(\mathcal{M})$. This induces the $C^\infty(\mathcal{M})$-linear musical isomorphism $P^\flat : \mathcal{X}^k(\mathcal{M}) \to \Omega^{n-k}_0(\mathcal{M})$ by $P^\flat(X) \equiv i_X P$, and we denoted its inverse by $P^\sharp$, $P^\sharp \circ P^\flat = Id [22]$ Sec. 2.5].

Note that since $P^\flat(X)$ is twisted, it is a form that takes value in the orientation line bundle. Since the orientation bundle is flat, we can find transition functions that are locally constant (in fact these are given by the sign of the Jacobian of the transition functions of $\mathcal{M}$). Hence the exterior derivative $\mathbf{d}$ on differential forms extend to an operator on twisted forms, which we will use in the definition of $\text{curl}_P$ below. Moreover $\mathbf{d}$ generates a canonical twisted de Rham complex by extending $\mathbf{d}$ using any trivialisation of the orientation line bundle induced by a trivialisation of $\mathcal{M}$, as explained in section 7 [27] (on orientable manifolds this reduces do the standard de Rham complex). Using this (extended) exterior derivative, we define the $P$-rotationnel as

$$\text{curl}_P = P^\sharp \circ \mathbf{d} \circ P^\flat,$$

which satisfies $\text{curl}_P \circ \text{curl}_P = 0$ since $\mathbf{d} \circ \mathbf{d} = 0$. In particular when applied to vector fields the $P$-rotationnel acts as the divergence operator $\text{curl}_P = \text{div}_P : \mathcal{X}(\mathcal{M}) \to C^\infty(\mathcal{M})$, which follows from

$$\mathcal{L}_X P = \mathbf{d} i_X P = P^\flat \text{curl}_P(X) = \text{curl}_P(X) P,$$

together with the definition of $\text{div}_P(X)$ as the function satisfying $\text{div}_P(X) P = \mathcal{L}_X P$. If $f$ is a function, observe that $(fP)^\flat = fP^\flat$, and so if $f$ is non-vanishing, $(fP)^\sharp = P^\sharp \circ \frac{1}{f}$. Hence

$$(51) \quad \text{curl}_{fP} = P^\sharp \circ \frac{1}{f} \circ \mathbf{d} \circ f \circ P^\flat \equiv P^\sharp \circ \mathbf{d}_f \circ P^\flat, \quad \text{or} \quad \text{curl}_{Qf} = P^\sharp \circ \mathbf{d} \frac{Qf}{\mathbf{d}f} \circ P^\flat,$$

where $\mathbf{d}_f \equiv \mathbf{d} + \mathbf{d} \log |f| \land$ is the distorted de Rham derivative. In particular, the $P$-rotationnel does not depend on the normalisation constant of $P$, an important requirement in many statistical applications, where the target distribution or statistical model is only known up to normalisation. Importantly, we have the following key result showing the homology groups defined by the boundary operator $\text{curl}_P$ (since $\text{curl}_P \circ \text{curl}_P = 0$) are isomorphic to the twisted de Rham cohomology groups. As usual we denote by $[\cdot]$ the equivalence classes.

**Theorem B.1.** The isomorphism $P^\flat$ descends to an isomorphism between the homology groups $\mathcal{H}_P(\mathcal{M})$ of $\text{curl}_P$ and the twisted de Rham cohomology groups.
$H_{dR}^{n-\ell}(M)$. Hence
\[
\text{Dyn}(P) \cong \text{curl}_P \left( X^{2}(M) \right) \oplus P^\ell \left( H_{dR}^{n-1}(M) \right),
\]
and any $P$-preserving dynamics will be globally the $P$-rotationnel of some $A \in X^2(M)$ iff the $(n-1)$ de twisted Rham cohomology is trivial. Moreover, if $U \subset M$ is an open subset, then $\text{curl}_P|_U = \text{curl}_P|_U$. Hence the set of $P$-preserving dynamics is precisely the set of locally $\text{curl}$ vector fields
\[
\text{Dyn}(P) = \text{Cur} \text{l}_{oc}(P)
\]
where $\text{Cur} \text{l}_{oc}(P) = \{X \in X(M) : \forall q, \text{there is a neighbourhood } U \text{ and } A \in X^2(U) s.t., X = \text{curli}_P|_U \}.$

**Proof.** The $P$-derivative $\text{curl}_P = P^\ell \circ d \circ P^\ell : X^k(M) \to X^{k-1}(M)$ is a vector space homomorphism, satisfying $\text{curl}_P \circ \text{curl}_P = 0$, that it is a boundary operator on the chain complex of $k$-multi-vector fields, and thus $\ker \left( \text{curl}_P : X^{k+1}(M) \to X^k(M) \right)$ is a linear subspace of $\ker \left( \text{curl}_P : X^{k+1}(M) \to X^k(M) \right)$. We can then define the $\ell$th Holomorphy group
\[
H^{\ell}_P(M) = \frac{\ker \left( \text{curl}_P : X^{\ell}(M) \to X^{\ell-1}(M) \right)}{\ker \left( \text{curl}_P : X^{\ell+1}(M) \to X^{\ell}(M) \right)}.
\]
and in particular the first one provides information on $P$-preserving vector fields (using $\text{curl}_P(X) = \text{div}_P(X)$)
\[
H^1_P(M) = \frac{\ker \left( \text{div}_P : X^1(M) \to C^\infty(M) \right)}{\ker \left( \text{curl}_P : X^2(M) \to X^1(M) \right)}.
\]
Notice that the map $[\cdot] \circ P^\ell : X^\ell(M) \to H^n_{dR}^{n-\ell}(M)$ descends to a map $H^{\ell}_P(M) \to H^{n-\ell}_{dR}(M)$, since $[\cdot] \circ P^\ell(X + \text{curl}_P(Y)) = [P^\ell(X)] + [d\text{curl}_P(Y)] = [P^\ell(X)]$. The map is surjective, since $\text{curl}_P : X^{k+1}(M) \to X^k(M)$ is a linear subspace of $\ker \left( \text{curl}_P : X^{k+1}(M) \to X^k(M) \right)$, and injective since $\ker \left( \text{curl}_P : X^{k+1}(M) \to X^k(M) \right) \cong \ker \left( \text{curl}_P : X^k(M) \to X^{k+1}(M) \right)$.

In general, we can still use Poincaré lemma (or Volterra theorem, as it was proved by Vito Volterra [157]) and the properties of $\text{curl}_P$ to show that any $P$-preserving vector field is locally a curl vector field. Denoting the inclusion by $\iota_U : U \to M$, we have $\iota_U^*(P^\ell(Y)) = \iota_U^*(i_Y P) = i_{\iota_U^*Y}\iota_U^*P = \iota_U^*P(Y_U)$, where $P_Y, Y_U$ denote their restriction to $U$, and we have used proposition 7.4.10 [2]; hence $\iota_U^* \circ P^\ell = P^\ell_U \circ |_U$. Setting $Y = P^\ell(\alpha)$ this yields $P^\ell(\alpha)|_U = P^\ell_U(\iota_U^*\alpha)$ for any twisted form $\alpha$. Hence
\[
|_U \circ \text{curl}_P \equiv |_U \circ P^\ell \circ d \circ P^\ell = P^\ell_U \circ |_U \circ d \circ P^\ell = P^\ell_U \circ d \circ P^\ell_U = P^\ell_U \circ |_U \circ \text{curl}_P(\alpha)
\]
Thus, $\text{curl}_P(Y) = 0$ iff $P^\ell \circ d \circ P^\ell(Y) = 0$ iff $d \circ P^\ell(Y) = 0$ (since $P^\ell$ is a linear isomorphism). By Poincaré Lemma, this holds iff around any point there is an open neighbourhood $U$ over which $P^\ell(Y)|_U = d\alpha$ for some twisted $(\dim(M) - 2)$-form $\alpha$ on $U$. Then $d\alpha = \iota_U^*(P^\ell(Y)) = P^\ell_U(Y_U)$, and $P^\ell_U(Y_U)|_U = d\alpha$ if $Y_U = P^\ell_U \circ |_U \circ \text{curl}_P(\alpha)$ where $\alpha \equiv P^\ell_U(\alpha)$ is a $2$-vector field on $U$.

Finally we also mention that when $P = dx$ is the Lebesgue measure on Euclidean space, $\text{Dyn}(dx) = \text{curl}_d x^2(M))$ was essentially already proved by Vito Volterra [157], that the statement $\text{Dyn}(P) \cong \text{curl}_P (X^2(M)) \oplus P^\ell (H_{dR}^{n-1}(M))$ appears in implicit form (essentially written as $P^\ell (\text{Dyn}(P)) = d\Omega^{n-2}(M) \oplus H^{n-1}(M)$ in [130] Thm. 6) under the assumption that $M$ is orientable, and that by Poincaré
If $M$ has a finite good cover (in which case the cohomology groups are finite dimensional) we may alternatively work with the first compactly supported de Rham cohomology group (proposition 5.3.1 and theorem 7.8 [27]). □

Note that by Poincaré duality if $M$ has a finite good cover we may alternatively work with the first compactly supported de Rham cohomology group. The de Rham cohomology groups may be very large, though they must be finite dimensional when $M$ is compact. Moreover, in that case, they are isomorphic to the vector spaces of harmonic forms, and the following results follows:

**Corollary B.2.** If $M$ is compact and orientable, then

$$\text{Dyn}(P) \cong \text{curl}_P \mathcal{X}^2(M) \oplus \mathcal{P}^2(\mathcal{H}^n-1(M)),$$

where $\mathcal{H}^n-1$ is the space of harmonic $n-1$-forms associated to an arbitrary Riemannian metric. In other words, any $P$-preserving vector field on a compact orientable manifold has the form $X = \text{curl}_P(\mathcal{A}) + \mathcal{P}^2(\gamma)$.

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