Barrier Hamiltonian Monte Carlo

Maxence Noble
Centre de Mathématiques Appliquées
Ecole Polytechnique, France
Institut Polytechnique de Paris

Valentin De Bortoli
Département d’Informatique
ENS, CNRS, Université PSL
Paris, France

Alain Durmus
Centre de Mathématiques Appliquées
Ecole Polytechnique, France
Institut Polytechnique de Paris

Abstract

In this paper, we propose Barrier Hamiltonian Monte Carlo (BHMC), a version of HMC which aims at sampling from a Gibbs distribution $\pi$ on a manifold $M$, endowed with a Hessian metric $g$ derived from a self-concordant barrier. Like Riemannian Manifold HMC, our method relies on Hamiltonian dynamics which comprise $g$. It incorporates the constraints defining $M$ and is therefore able to exploit its underlying geometry. We first introduce c-BHMC (continuous BHMC), for which we assume that the Hamiltonian dynamics can be integrated exactly, and show that it generates a Markov chain for which $\pi$ is invariant. Secondly, we design n-BHMC (numerical BHMC), a Metropolis-Hastings algorithm which combines an acceptance filter including a “reverse integration check” and numerical integrators of the Hamiltonian dynamics. Our main results establish that n-BHMC generates a reversible Markov chain with respect to $\pi$. This is in contrast to existing algorithms which extend the HMC method to Riemannian manifolds, as they do not deal with asymptotic bias. Our conclusions are supported by numerical experiments where we consider target distributions defined on polytopes.

1 Introduction

Markov Chain Monte Carlo (MCMC) methods is one of the primary algorithmic approaches to obtain approximate samples from a target distribution $\pi$. Indeed, they have been successively applied over these past decades in a large panel of practical settings, (Liu and Liu, 2001). In particular, gradient-based MCMC methods have shown their efficiency and robustness in high-dimensional settings, and come nowadays with important theoretical guarantees (Dalalyan, 2017; Durmus and Moulines, 2017). However, they still struggle in facing the case where the target distribution is supported on a constrained subset $M$ of $\mathbb{R}^d$, (Gelfand et al., 1992; Pakman and Paninski, 2014; Lan and Shahbaba, 2015). Yet, this problem appears in various fields; see e.g., (Morris, 2002; Lewis et al., 2012; Thiele et al., 2013) for some specific applications in computational statistics and biology.

Drawing samples from such distributions is indeed a challenging problem that has been intensively studied in the literature, (Dyer and Frieze, 1991; Lovász and Simonovits, 1993; Lovász and Kannan, 1999; Lovász and Vempala, 2007; Brubaker et al., 2012; Cousins and Vempala, 2014; Pakman and Paninski, 2014; Lan and Shahbaba, 2015; Bubeck et al., 2015). In particular, some recent extensions of the popular Metropolis-Hastings (MH) algorithm to constrained spaces consist in designing proposals based on dynamics for which $\pi$ is invariant, (Zappa et al., 2018; Lelièvre et al., 2019, 2022). In practice, the corresponding solutions are numerically integrated based on implicit and symplectic schemes, which however come with new difficulties. As first observed by Zappa et al. (2018), an additional “reverse integration check“ in the usual MH filter is necessary to ensure that the resulting Markov kernel admits $\pi$ as a stationary distribution.

In this paper, we aim at generalizing this family of methods taking into account the geometry of the constrained subspace, building on the Riemannian Manifold Hamiltonian Monte Carlo (RMHMC) algorithm introduced by Girolami and Calderhead (2011). Similarly to HMC, (Duane et al., 1987; Neal et al., 2011; Betancourt, 2017), RMHMC aims to target a positive distribution $\pi$ on $\mathbb{R}^d$ and relies on the integration of a canonical Hamiltonian equation. In contrast, RMHMC incorporates some geometrical information in the definition of the Hamiltonian via a Riemannian metric $g$ on $\mathbb{R}^d$. When considering applications of RMHMC to a convex, open and bounded subset $M$, a natural choice for this metric is the Hessian metric associated with a self-concordant barrier on $M$, (Nesterov and Nemirovskii, 1994), as suggested by Kook et al. (2022). We adopt here the same approach and now focus on a constrained subspace $M$ which is supposed to be equipped with an appropriately designed “self-concordant” metric, (Nesterov and Nemirovskii, 1994).
Considering this setting, we propose BHMC (Barrier HMC). To the best of our knowledge, this is the first version of RHMHMC incorporating a "reverse integration check". We present two versions of BHMC, c-BHMC and n-BHMC, which differ by their ability of exactly computing the Hamiltonian dynamics. For each algorithm, we prove that the generated Markov chain preserves \( \pi \).

**Outline of the work.** The rest of the paper is organized as follows. In Section 2, we introduce our sampling framework and review some background on self-concordance and Riemannian geometry. In Section 3, we propose c-BHMC and prove its reversibility. In Section 4, we present n-BHMC and its main components, for which we derive theoretical results in Section 5. We review related works in Section 6 and provide numerical experiments in Section 7. Finally, we conclude with some perspectives in Section 8.

**Notation.** For any \( f \in C^3(\mathbb{R}^d, \mathbb{R}) \), we denote by \( Df \) (and \( D^2 f \)) the Jacobi (respectively the Hessian) of \( f \). For any matrix \( A \in \mathbb{R}^{d \times d} \) and any \( x \in \mathbb{R}^d \), we denote by \( A : D^3 f(x) \) the vector \( (\text{Tr}(A^T \{ D^3 f(x) \}_i))_{i \in [d]} \). For any positive-definite matrix \( \lambda \in \mathbb{R}^{d \times d} \), \( \langle \cdot , \cdot \rangle_\lambda \) stands for the scalar product induced by \( \lambda \) on \( \mathbb{R}^d \), defined by \( \langle x, y \rangle_\lambda = \langle x, Ay \rangle \). The "momentum reversal" operator \( s : \mathbb{R}^d \times \mathbb{R} \to \mathbb{R}^d \times \mathbb{R} \) is defined for any \( (x,p) \in \mathbb{R}^d \times \mathbb{R} \) by \( s(x,p) = (x,-p) \). Let \( E,F \) be two sets and \( h : E \to 2^G \), where \( G \) is the set of sets of \( F \). We say that \( h \) is a set-valued map. Note that any map \( g : E \to F \) can be extended to a set-valued map by identifying, for any \( x \in E \), \( g(x) \) and \( \{ g(x) \} \). Let \( f : F \to 2^G \). We define \( f \circ h : E \to 2^G \) for any \( x \in E \) by \( f \circ h(x) = \cup_{y \in h(x)} f(y) \), where by convention \( \cup_\emptyset = \emptyset \). For any topological space \( X \), we denote \( B(X) \) its Borel sets. Finally, for any probability measure \( \mu \in \mathcal{P}(X) \) and measurable map \( \varphi : X \to Y \), we denote \( \varphi \# \mu \in \mathcal{P}(Y) \) the pushforward of \( \mu \) by \( \varphi \). In general, we will equivalently denote by \( \varphi \# \mu \) a state of the Hamiltonian system.

### 2 Setting and Background

In this paper, we consider an open subset \( M \subset \mathbb{R}^d \), and we aim at sampling from a target distribution \( \pi \) given for any \( x \in M \) by

\[
\frac{d\pi(x)}{dx} = \exp[-V(x)]/Z ,
\]

where \( V \in C^2(M, \mathbb{R}) \) and \( Z = \int_M \exp[-V(x)]dx \). We view here \( M \) as an embedded submanifold of \( \mathbb{R}^d \), equipped with a metric \( g \), satisfying the following assumptions.

**A1.** \( M \) is an open convex bounded subset of \( \mathbb{R}^d \).

**A2.** There exists \( \phi \), a \( \alpha \)-regular and \( \nu \)-self-concordant barrier on \( M \) (see Definitions 1 and 13) such that \( g = D^2 \phi \).

We provide in Section 2.1 basic Riemannian facts along with the definition of the Hamiltonian dynamics of R MHMC and introduce self-concordance in Section 2.2.

#### 2.1 Riemannian Manifold Hamiltonian dynamics

**Basics on Riemannian geometry.** Let \( M \) be a \( d \)-dimensional smooth manifold, endowed with a metric \( g \). We recall that the Riemannian volume element corresponding to \( (M, g) \) is given in local coordinates by

\[
\text{dvol}_M(x) = \sqrt{\det(g)}dx ,
\]

where \( dx \) is a dual coframe, (Lee, 2006, Lemma 3.2.).

We denote by \( T^*_xM \) the dual of the tangent space at \( x \in M \), i.e., the cotangent space. For any \( x \in M \), \( T^*xM \) is a vector space naturally endowed with the scalar product \( \langle \cdot , \cdot \rangle_{g(x)^{-1}} \) (Mok, 1977). We recall that the cotangent bundle \( T^*M \) is defined by \( T^*M = \cup_{x \in M} \{ x \} \cup T^*_xM \). This set is a \( 2d \)-dimensional manifold endowed with a Riemannian metric \( g^* \) given by Mok (1977) inherited from \( g \). With this metric, the volume form on \( T^*M \) satisfies for any \( (x,p) \in T^*M \)

\[
\text{dvol}_{T^*M}(x,p) = dx dp ,
\]

where \( dx dp \) is a dual coframe for \( T^*M \).

Therefore, under A1., identifying \( T^*M \) with \( \mathbb{R}^{2d} \), the volume form on \( T^*M \) is the Lebesgue measure of \( \mathbb{R}^d \times \mathbb{R}^d \) restricted to \( T^*M \). We refer to Appendix B for details on the cotangent bundle and its metric \( g^* \).

**Hamiltonian dynamics.** Note that with the previously introduced notation, \( \pi \) can be expressed as

\[
\pi(x)/\text{dvol}_M(x) = \exp[-V(x) - \frac{1}{2} \log(\det(g(x)))]/Z .
\]

This motivates the introduction of the following Hamiltonian on \( T^*M \)

\[
H(x,p) = V(x) + \frac{1}{2} \log(\det g(x)) + \frac{1}{2} ||p||^2_{g(x)^{-1}} .
\]

In this definition, we notably take into account the scalar product \( \langle \cdot , \cdot \rangle_{g(x)^{-1}} \) on \( T^*_xM \). Finally, we consider the joint distribution \( \bar{\pi} \) on \( T^*M \)

\[
\bar{\pi}(x,p) = (1/\bar{Z}) \exp[-H(x,p)]\text{dvol}_{T^*M}(x,p) ,
\]

where \( \bar{Z} = \int_{T^*M} \exp[-H(x,p)]\text{dvol}_{T^*M}(x,p) \) for which the first marginal is \( \pi \). Indeed, for any \( \varphi \in C(M, \mathbb{R}) \)

\[
\int_{T^*M} \varphi(x)\text{d\bar{\pi}}(x,p) = \int_{T^*M} \varphi(x)\text{d\pi}(x)N_x(p,0,Id)dp = \int_M \varphi(x)\text{d\pi}(x) ,
\]

where we denote by \( N_x(0,0) \) the centered standard Gaussian distribution w.r.t. \( \| \cdot \|_{g(x)^{-1}} \). The Hamiltonian dynamics associated with \( H \) is given by the following ODEs

\[
\dot{x} = \partial_p H(x,p), \quad \dot{p} = -\partial_x H(x,p) ,
\]

where the derivatives of \( H \) can be computed explicitly as

\[
\partial_p H(x,p) = g(x)^{-1} p, \quad \partial_x H(x,p) = -\frac{1}{2} Dg(x)[g(x)^{-1} p, g(x)^{-1} p] + L(x) ,
\]

where \( L(x) = \nabla V(x) + \frac{1}{2} g(x)^{-1} : Dg(x) \).
2.2 Self-concordance and regularity

Until now, we have considered an arbitrary Riemannian metric \( g \). In the rest of this work, we focus on metrics given by Hessian of self-concordant barriers.

**Self-concordance.** We first introduce self-concordant barriers, a family of smooth convex functions which are well-suited for minimization by the Newton method.

**Definition 1** (Nesterov and Nemirovskii (1994)). Let \( U \) be a non-empty open convex domain in \( \mathbb{R}^d \). A function \( \phi : U \to \mathbb{R} \) is said to be a \( \nu \)-self-concordant barrier (with \( \nu \geq 1 \)) on \( U \) if it satisfies:

(a) \( \phi \in C^3(U, \mathbb{R}) \) and \( \phi \) is convex,
(b) \( \phi(x) \to +\infty \) as \( x \to \partial U \),
(c) \( |D^3 \phi(x)[h, h, h]| \leq 2\|h\|\|\nabla \phi(x)\|_g, \) for any \( x \in M, h \in \mathbb{R}^d \),
(d) \( |D^2 \phi(x)[h]|^2 \leq \nu \|h\|^2_\|g(x)\|, \) for any \( x \in M, h \in \mathbb{R}^d \),

where \( g(x) = D^2 \phi(x) \).

Balls for \( \|\cdot\|_g(x) \) are called Dikin ellipsoids and are central for the study of self-concordance, see Appendix C.

**Regularity.** The property of \( \alpha \)-regularity for some \( \alpha \geq 1 \) is shared by many self-concordant barriers, including logarithmic and quadratic programming barriers. It ensures stability for interior point polynomial methods. Definition and properties of \( \alpha \)-regularity are recalled in Appendix C.

**Example of the polytope.** Let us assume that \( M \) is the polytope \( M = \{x : Ax < b\} \), where \( A \in \mathbb{R}^{m \times d} \) and \( b \in \mathbb{R}^m \). We endow it with the Riemannian metric \( g(x) = D^2 \phi(x) \) where \( \phi : M \to \mathbb{R} \) is the logarithmic barrier given for any \( x \in M \) by \( \phi(x) = -\sum_{i=1}^m \ln(b_i - A_i^\top x) \). The barrier \( \phi \) is both a \( m \)-self-concordant barrier and a 2-regular function, (Nesterov and Nemirovskii, 1998, page 3). Moreover, we have for any \( x \in M \), \( g(x) = A^\top S(x)^{-2}A \), where \( S(x) = \text{Diag}(b_i - A_i^\top x) \in \mathbb{R}^m \). We provide in Figure 1 an illustration of this barrier.

3 c-BHMC: Algorithm and Results

We first state general results on the Hamiltonian dynamics (3) under our main assumptions. It allows us to introduce the **continuous** version of BHMC (c-BHMC), for which we derive the reversibility with respect to \( \pi \). Proofs of this section are postponed to Appendix D.

**Results on the Hamiltonian dynamics.** We present below the existence and uniqueness of the Hamiltonian dynamics (3), given a starting point \( z_0 \in T^*M \).

**Proposition 2.** Assume \( A_1, A_2 \). Let \( z_0 \in T^*M \), then (3) admits a unique maximal solution \( (J_{z_0}, z) \), where (i) \( J_{z_0} \subset \mathbb{R} \) is an open neighbourhood of 0, (ii) \( z \in C^1(J_{z_0}, T^*M) \), (iii) \( z(0) = z_0 \) and (iv) for any \( t \in J_{z_0}, H(z(t)) = H(z_0) \).

In addition, we can characterize the Hamiltonian dynamics if they explode in finite time.

**Proposition 3.** Assume \( A_1, A_2 \). Let \( z_0 \in T^*M \), \( (J_{z_0}, z) \) as in Proposition 2. If \( T_{z_0} = \sup J_{z_0} < +\infty \), then

- \( \lim_{t \to T_{z_0}} ||p(t)|| = +\infty \).
- There exists \( x_M \in \partial M \) such that \( \lim_{t \to T_{z_0}} x(t) = x_M \).

**Algorithm 1 c-BHMC with Momentum Refresh**

1: HMC Input: \( (x_0, p_0) \in T^*M, \beta \in (0, 1], N \in \mathbb{N} \)
2: ODE Input: \( h \)
3: Output: \( (x_n, p_n)_{n \in \mathbb{N}} \)
4: for \( n = 1, \ldots, N \) do
5: \( x, p \leftarrow x_{n-1}, p_{n-1} \)
6:  Step 1: \( \tilde{p} \sim N_z(0, \text{Id}), \tilde{p} \leftarrow \sqrt{1 - \beta \tilde{p} + \beta \tilde{p}} \)
7:  Step 2: solving continuous ODE (3)
8:  \( \text{if } z \in E_h \text{ then} \)
9:  \( (x_n, p_n) \leftarrow T_h(z) \)
10:  \text{else}
11:  \( (x_n, p_n) \leftarrow s(z) \)
12:  Step 3: \( \tilde{p} \sim N_z(0, \text{Id}), \tilde{p} \leftarrow \sqrt{1 - \beta \tilde{p} + \beta \tilde{p}} \)

**Introduction to c-BHMC.** Motivated by Proposition 2, we define, for any \( h > 0 \), the set \( E_h \subset T^*M \)

\[ E_h = \{ z \in T^*M : h < \sup J_z \} \],

and the map \( T_h : E_h \to T^*M \) such that \( T_h(z_0) = z(h) \) for any \( z_0 \in T^*M \), \( z \) being uniquely defined in Proposition 2. Note that \( T_h(z_0) \) computes exactly the Hamiltonian dynamics on a time interval \( [0, h] \), starting at \( z_0 \).

We also define for any \( h > 0 \) the set \( E_h \subset T^*M \) which will ensure that Hamiltonian dynamics computed in c-BHMC are reversible

\[ E_h = \{ z \in E_h : h < \sup J_z \} \].

The algorithm then proceeds as follows. First, sample a new momentum \( \tilde{p} \) with momentum refresh \( \beta \). Then, if the obtained point \( (x, p) \) is in \( E_h \), follow the Hamiltonian dynamics (3) with starting point \( (x, p) \) up until time \( h \); otherwise, switch the momentum. Finally, refresh the momentum as in the beginning of the iteration. The full algorithm is described in Algorithm 1.
Denote by \( Q_c : T^*M \times B(T^*M) \to [0, 1] \), the transition kernel of the (homogeneous) Markov chain \( (x_n, p_n)_{n \in [N]} \) generated by Algorithm 1. Using the properties of the Hamiltonian dynamics, we get the following result.

**Theorem 4.** Assume A1, A2. Then, \( Q_c \) is reversible up to momentum reversal, i.e., we have for any \( f \in C(T^*M \times T^*M, \mathbb{R}) \) with compact support

\[
\int_{T^*M \times T^*M} f(z, z')d\pi(z)Q_c(z, dz') = \int_{T^*M \times T^*M} f(s(z'), s(z))d\pi(z)Q_c(z, dz') .
\]

In particular, \( \pi \) is an invariant measure for \( Q_c \).

## 4 Presentation of n-BHMC

In practice, it is not possible to exactly compute the Riemannian Hamiltonian dynamics \((3)\). We thus introduce a numerical version of BHMC (n-BHMC) in which we replace the continuous ODE integration by a symplectic numerical scheme. We first define the Hamiltonian integrators used in n-BHMC in Section 4.1 and then provide details on the different steps of n-BHMC in Section 4.2.

### 4.1 Hamiltonian integrators of n-BHMC

In the same spirit as Shahbaba et al. (2014), we first rewrite the Hamiltonian \( H \) given in \((1)\) as \( H = H_1 + H_2 \), where we highlight the non separable aspect of \( H \) in \( H_2 \), i.e., for any \((x, p) \in T^*M \)

\[
H_1(x, p) = V(x) + \frac{1}{2}\log(\det g(x)) ,
\]

\[
H_2(x, p) = \frac{1}{2}\|p\|^2_{g(x)^{-1}} .
\]

Therefore, we have

\[
\partial_x H_1(x, p) = L(x), \quad \partial_p H_1(x, p) = 0 ,
\]

\[
\partial_x H_2(x, p) = -\frac{1}{2}Dg(x)[g(x)^{-1}p, g(x)^{-1}p] ,
\]

\[
\partial_p H_2(x, p) = g(x)^{-1}p ,
\]

where \( L(x) = \nabla V(x) + \frac{1}{2}g(x)^{-1} : Dg(x) \). Leveraging the separable structure of \( H_1 \) we now define an implicit scheme to discretize the Hamiltonian dynamics.

**Explicit integrator of \( H_1 \).** For any \( h \in \mathbb{R} \), we define the map \( S_{h/2} : T^*M \to T^*M \), which approximates the dynamics of \( H_1 \) on a step-size \( h/2 \)

\[
S_{h/2}(x, p) = (x, p - \frac{h}{2}\partial_x H_1(x, p)) .
\]

We have: (i) \( S_{h/2}(T^*M) \subset T^*M \), (ii) \( S_{h/2} \) is symplectic (we refer to Appendix E for more details on symplecticity), (iii) \( S_{-h/2} \circ S_{h/2} = \text{Id} \) and \( S_{h/2} \circ S_{-h/2} = \text{Id} \) and (iv) \( S_{-h/2} = s \circ S_{h/2} \circ s \). Note that \( s \circ S_{h/2} \) is an involution on \( T^*M \), which inherits from properties (i) and (ii) of \( S_{h/2} \).

**Implicit integrator of \( H_2 \).** We denote by \( F_h \) the set-valued map defined on \( T^*M \) by \( F_h = G_h \circ s \), where \( G_h \) is a fixed implicit second-order integrator of Hamiltonian \( H_2 \) with step-size \( h \). For theoretical purposes we focus on the Störmer-Verlet scheme, (Hairer et al., 2006, Theorem VI.3.4.), also known as the generalized Leapfrog integrator. This integrator is widely used in geometric integration, (Girolami and Calderhead, 2011; Betancourt, 2013; Cobb et al., 2019; Brofos and Lederman, 2021a) and we refer to Appendix E for a discussion of other numerical schemes.

For any \((z^{(0)}, z^{(1)}) \in T^*M \times T^*M \), \( z^{(1)} = (x^{(1)}, p^{(1)}) \in G_h(z^{(0)}) \) if \( z^{(1)} \) solves the following system

\[
p^{(1/2)} = p^{(0)} - \frac{h}{2}\partial_z H_2(x^{(0)}, p^{(1/2)}) ,
\]

\[
x^{(1)} = x^{(0)} + \frac{h}{2}[\partial_p H_2(x^{(0)}, p^{(1/2)}) + \partial_p H_2(x^{(1)}, p^{(1/2)})] ,
\]

\[
p^{(1)} = p^{(1/2)} - \frac{h}{2}\partial_z H_2(x^{(1)}, p^{(1/2)}) .
\]

The integrator \( G_h \) is a set-valued map which satisfies:

(i) \( G_h(T^*M) \subset 2T^*M \), (ii) \( G_{-h} = s \circ G_h \circ s \), since \( \partial_p H_2(s(z)) = -\partial_p H_2(z) \) and \( \partial_z H_2(s(z)) = \partial_z H_2(z) \), (iii) if \( |G_h(z)| > 0 \) then \( z \in G_{-h} \circ G_h(z) \). As a result, \( F_h \) enjoys similar properties. We emphasize that the set-valued-map \( F_h \circ s = G_h \) approximates the dynamics of the Hamiltonian \( H_2 \) with a step-size \( h \). We also define the set-valued map \( R_h : T^*M \to T^*M \)

\[
R_h = (s \circ S_{h/2}) \circ F_h \circ (s \circ S_{h/2}) ,
\]

and emphasize that the set-valued map \( s \circ R_h \) approximates the dynamics of the Hamiltonian \( H \) with a step-size \( h \).

**Numerical integrator of \( H_2 \).** In practice, we do not have access to \( F_h \) but approximate it with a numerical map \( \Phi_h \). This integrator is defined on a domain \( \text{dom} \Phi_h \subset T^*M \) with \( \Phi_h(\text{dom} \Phi_h) \subset T^*M \). We also define the numerical map \( R^\Phi_h : (s \circ S_{h/2})(\text{dom} \Phi_h) \subset T^*M \to T^*M \)

\[
R^\Phi_h = (s \circ S_{h/2}) \circ \Phi_h \circ (s \circ S_{h/2}) .
\]

Similarly to \( R_h \), \( s \circ R^\Phi_h \) approximates the dynamics of Hamiltonian \( H \) on a step-size \( h \). In our experiments, we design \( \Phi_h \) using a fixed-point solver with a given number of iterations following Brofos and Lederman (2021a,b). We refer to Appendix I for details on computations of \( \Phi_h \).

### 4.2 The n-BHMC algorithm

We are now ready to detail the different steps of n-BHMC which is presented in Algorithm 2.

**Steps 1 and 5: applying a momentum update.** Given a current state \((x, p) \in T^*M \), the momentum is updated as \( p \leftarrow \sqrt{1 - \beta^2}p + \sqrt{\beta Z} \), where \( Z \sim N_p(0, 1d) \), for some refresh parameter \( \beta \in (0, 1] \). This update is applied both at the beginning and the end of the iteration, similarly to Lelièvre et al. (2022).

\footnote{Note that \( s \circ R^\Phi_h \) is a function and not a set-valued map.}
Algorithm 2 n-BHMC with Momentum Refresh

1: HMC Input: \((x_0, p_0) \in T^*\mathcal{M}, \beta \in (0, 1], N \in \mathbb{N}\)
2: ODE Input: \(h, \eta, \Phi_h\) with domain \(\text{dom}\Phi_h\)
3: Output: \((x_n, p_n)_{n \in \mathbb{N}}\)
4: for \(n = 1, \ldots, N\) do
5: \(x, p \leftarrow x_{n-1}, p_{n-1}\)
6: \(\text{Step 1: } \hat{p} \sim \mathcal{N}_z(0, \text{Id}), p \leftarrow \sqrt{1-\beta}p + \sqrt{\beta}\hat{p}\)
7: \(\text{Step 2: solving discretized ODE (3)}\)
8: \(x', p' \leftarrow \Phi_h(z(0))\)
9: \(x^{(0)}, p^{(0)} \leftarrow (s \circ S_{h/2})(x, p)\)
10: if \(z(0) \in \text{dom}\Phi_h\) then
11: \(z(1) = \Phi_h(z(0))\)
12: \(\text{error}_0 = \|z(0) - \Phi_h(z(1))\|_{z(0)}\)
13: \(\text{error}_1 = \|z(0) - \Phi_h(z(1))\|_{\Phi_h(z(1))}\)
14: \(\text{if } z(1) \in \text{dom}\Phi_h \& \text{error}_0 \leq \eta \text{ then } x', p' \leftarrow (s \circ S_{h/2})(x^{(1)}, p^{(1)})\)
15: \(\text{Step 3: } a \leftarrow \min(1, \exp[-H(x', p') + H(x, p)])\)
16: \(u \sim U[0, 1]\)
17: if \(u \leq a\) then
18: \(\tilde{x}, \tilde{p} \leftarrow x', p'\)
19: else
20: \(\tilde{x}, \tilde{p} \leftarrow x, p\)
21: \(\text{Step 4: } x_n, p_n \leftarrow s(\tilde{x}, \tilde{p})\)
22: \(\text{Step 5: } \hat{p} \sim \mathcal{N}_z(0, \text{Id}), p_n \leftarrow \sqrt{1-\beta}\tilde{p} + \sqrt{\beta}\hat{p}\)

Step 2: solving discretized ODE (3). We now solve the discretized dynamics of \(H\) with a step-size \(h\), starting from \((x, p)\), while ensuring that the proposal state belongs to \(T^*\mathcal{M}\). We proceed as follows:

(a) Starting from \((x, p)\), we first run the explicit integrator \(S_{h/2}\), which encodes Hamiltonian \(H_1\) with step-size \(h/2\), and compute \(z(0) = (s \circ S_{h/2})(x, p)\).

(b) If \(z(0)\) is not in the domain of \(\Phi_h\), i.e., \(z(0) \notin \text{dom}\Phi_h\), then \((x', p')\) is not updated and we directly go to Step 3. If \(z(0) \in \text{dom}\Phi_h\), we define \(z(1) = \Phi_h(z(0))\) as an approximation of the Hamiltonian dynamics \(H_2\). To ensure the reversibility of this step, we perform a “reverse integration check” (Zappa et al., 2018; Lelièvre et al., 2019), i.e., we verify (a) \(z(1) \in \text{dom}\Phi_h\) and (b) \(z(0) = \Phi_h(z(1))\). In practice, we replace condition (b) with an explicit tolerance threshold \(\eta\) and reject the proposal if

\[
\|z(0) - \Phi_h(z(1))\|_{z(0)} + \|z(0) - \Phi_h(z(1))\|_{\Phi_h(z(1))} > \eta,
\]

where, for any \(z, z' \in T^*\mathcal{M}\), we define on \(T^*\mathcal{M}\) the norm \(\| \cdot \|_{z}\) by \(\|z'\|_{z} = \|z'\|_{g(z)} + \|p'\|_{g(z^{-1})}\). We discuss the choice of this norm to perform the “reverse integration check” and compare it with the Euclidean norm in Section 7.

An illustration of failures of condition (a) and condition (b) is given in Figure 2. If both of these conditions are satisfied, we finally set \((x', p') = (s \circ S_{h/2})(z(1))\), to ensure the reversibility of the update of \((x', p')\). Otherwise, \((x', p')\) is not updated and we go to Step 3.

Step 3: computing the acceptance filter. We denote by \(a(x', p'|x, p)\) the acceptance probability to move from \((x, p) \in T^*\mathcal{M}\) to \((x', p') \in T^*\mathcal{M}\), which is given by

\[
a(x', p'|x, p) = 1 \wedge \exp[-H(x', p') + H(x, p)].
\]

After Step 2, we perform a simple MH filter by accepting the proposal with probability \(a(x', p'|x, p)\) similar to a classical HMC algorithm. We emphasize that there are four cases under which the state \((x, p)\) is not updated:

(a) \(z(0) \notin \text{dom}\Phi_h\) (there is no numerical solution of the discretized ODE of Hamiltonian \(H_2\) starting from \(z(0)\)),

(b) \(z(0) \in \text{dom}\Phi_h\) but \(\Phi_h(z(0)) \notin \text{dom}\Phi_h\),

(c) \(z(0) \in \text{dom}\Phi_h\) and \(\Phi_h(z(0)) \in \text{dom}\Phi_h\), but \(\Phi_h \circ \Phi_h(z(0)) \neq z(0)\),

(d) We reject the move with the MH filter.

Step 4: applying momentum reversal. To ensure a move along the Hamiltonian \(H\) with step-size \(h\), we reverse the momentum after the acceptance step. Indeed, if the acceptance filter is successful, then \((x_n, p_n) = (s \circ R_{h}^p)(x_{n-1}, p_{n-1})\) approximates the Hamiltonian dynamics with a step-size \(h\) starting at \((x_{n-1}, p_{n-1})\) as seen in Section 4.1. Otherwise, \((x_n, p_n) = (x_{n-1}, -p_{n-1})\).

5 Main Results

In this section, we study the reversibility of n-BHMC with respect to the target distribution. In Section 5.1 we first prove symplectic properties for the implicit map \(F_h\). More precisely, we show in Proposition 3 that even though \(F_h\) is a set-valued map, it can locally be identified with a \(C^1\)-diffeomorphism. In a manner akin to Lelièvre et al. (2022), this result thus justifies our assumption that the numerical map \(\Phi_h\) used to approximate \(F_h\) in the Step 2 of Algorithm 2 is locally a \(C^1\)-involution.
As explained in Section 5.2, this last assumption is however not enough to prove the reversibility of n-BHMC. To do so, we slightly modify Algorithm 2, by introducing a tighter condition in the “reverse integration check”. We refer to Algorithm 3 in Appendix G for a presentation of this new version of n-BHMC. Finally, we prove in Theorem 6 that this algorithm is reversible with respect to \( \pi \).

5.1 From implicit to numerical integrators

**Proposition 5.** Assume A1, A2. Let \( z^{(0)} \in T^{*}M \), then there exists \( h^{*} \geq 0 \) (explicit in Appendix F) such that for any \( h \in (0, h^{*}) \), there exist \( z^{(1)}_{h} \in F_{h}(z^{(0)}) \), a neighborhood \( U \subset T^{*}M \) of \( z^{(0)} \) and a \( C^{1} \)-diffeomorphism \( \gamma_{h} : U \rightarrow \gamma_{h}(U) \subset T^{*}M \) with

(a) \( \gamma_{h}(z^{(0)}) = z^{(1)}_{h} \) and \( | \det \text{Jac}(\gamma_{h}) | = 1 \).

(b) \( \gamma_{h}(z) \) is the only element of \( F_{h}(z) \) in \( \gamma_{h}(U) \) for \( z \in U \).

Proposition 5 shows that while \( F_{h} \) can take multiple (or none) values on \( T^{*}M \), for any \( z^{(0)} \in T^{*}M \), there exist \( h \) small enough and a neighborhood \( U \) of \( z^{(0)} \) such that the set-valued map \( F_{h} \) contains a \( C^{1} \)-diffeomorphism on \( U \). The proof of Proposition 5 is postponed to Appendix F.

Motivated by this result on the implicit map \( F_{h} \) and the fact that for any \( z \in T^{*}M \) with \( |F_{h}(z)| > 0, z \in F_{h} \circ F_{h}(z) \), see Section 4.1, we make the following assumption on the numerical map \( \Phi_{h} \).

**A3.** There exists \( \lambda \in (0, 1) \) such that for any \( z^{(0)} \in T^{*}M \), there exists \( h_{*} \) such that for any \( h \in (0, h_{*}) \),

(a) \( B = B_{\| \cdot \|_{\infty}}(z^{(0)}, \lambda r_{z^{(0)}}) \subset \text{dom} \Phi_{h} \),

(b) \( \Phi_{h} \in C^{1}(B, T^{*}M) \) and \( \Phi_{h} \circ \Phi_{h} = \text{Id} \) on \( B \),

with \( r_{z^{(0)}} \) depending only on \( g \) and defined in Appendix H.

A3 can be thought as a strengthening of Proposition 5-(a), where (i) \( h_{*} \) refers to \( h^{*} \), and (ii) \( B \) and \( \Phi_{h} \) correspond to explicit versions of \( U \) and \( \gamma_{h} \).

Finally, we conjecture that the involution condition in A3-(b) could in fact be replaced by the condition that for any \( z \in B, \Phi_{h}(z) \in F_{h}(z) \), in a manner akin to Lelièvre et al. (2022). We leave this study for future work.

5.2 Reversibility results

**Beyond n-BHMC.** While Algorithm 2 can be implemented practically, it cannot be easily analysed under A1, A2 and A3. The main reason for this limitation is that we cannot ensure that \( \Phi_{h} \) is locally an involution around \( z^{(0)} \) if \( h \approx h_{*} \). To circumvent this issue we enforce a condition on \( h \) to be small enough in n-BHMC. This yields a straightforward modification of Algorithm 2 presented in Algorithm 3, see Appendix G. Namely, we replace the condition that iterates stay on the domain of \( \Phi_{h} \) and the “reverse integration check” (Step 2 of Algorithm 2) by a condition on \( h \) (Step 2 of Algorithm 3). This alternative check is more restrictive but allows us to prove the reversibility of the algorithm.

We denote by \( Q : T^{*}M \times B(T^{*}M) \rightarrow [0, 1] \), the transition kernel of the Markov chain \( \{x_{n}, p_{n}\}_{n \in [N]} \) generated by Algorithm 3. We now state our main result, whose proof is provided in Appendix H.

**Theorem 6.** Assume A1, A2, A3. Then, \( Q \) is reversible up to momentum reversal, i.e., we have for any \( f \in C(T^{*}M \times T^{*}M, \mathbb{R}) \) with compact support \( f \)

\[
\int_{T^{*}M} f(z, z') \bar{\pi}(z) \, dz \, dz' = \int_{T^{*}M} f(s(z'), s(z)) \bar{\pi}(z) \, dz \, dz'.
\]

**Proof.** We provide here a sketch of the proof, details being postponed to the appendix. The reversibility (up to momentum reversal) of the momentum update is straightforward. To establish the reversibility up to momentum reversal of the numerical Hamiltonian integration step, we cover the compact support of \( f \) with a finite family of open balls with respect to the metric \( g \). Combining A2 and A3, we show that \( \Phi_{h} \) is an involution on each one of these sets. We then conclude upon combining this result with the fact that \( R_{h}^{\lor} \circ S_{h/2} = s \circ S_{h/2} \circ \Phi_{h} \).

6 Related work

**Sampling on manifolds.** Traditional constrained sampling methods in Euclidean spaces include the Hit-and-Run algorithm (Lovász and Vempala, 2004), the Random Walk Metropolis-Hastings (RWMH) algorithm, also referred to as Ball Walk (Lee and Vempala, 2017b), and HMC, (Duane et al., 1987). However, it has been empirically demonstrated that RWMH and HMC require small step-sizes in order to correctly sample from a target distribution \( \pi \) over a submanifold \( M \subset \mathbb{R}^{d} \), thus resulting in poor mixing time (Girolami and Calderhead, 2011, Figures 1 and 3). In the specific case where \( M = \{ x \in \mathbb{R}^{d} : c(x) = 0 \} \) for some \( c : \mathbb{R}^{d} \rightarrow \mathbb{R}^{m} \), Brubaker et al. (2012) combine HMC with the RATTLE integrator (Leimkuhler and Skeel, 1994), incorporating the constraints of \( M \) in the Hamiltonian dynamics via Lagrange multipliers.

Girolami and Calderhead (2011) adopt an original approach by endowing \( M \) with a Riemannian metric \( g \) and propose RMHMC (Riemannian Manifold Hamiltonian Monte Carlo), a version of HMC where the Hamiltonian depends on \( g \) as in (1). Their method consists of integrating the Hamiltonian dynamics of (3) on short-time steps.
using the generalized Leapfrog integrator (4) and the acceptance filter defined in (6). This method does not include a “reverse integration check” (Line 14 in Algorithm 2), and therefore the reversibility of the algorithm cannot be ensured in practice. In a similar line of work, Byrne and Girolami (2013) propose to design a numerical integrator for RMHMC using geodesics.

**Choice of the metric.** There are various ways to design a meaningful metric $g$ given a submanifold $M$. In a Bayesian perspective, Girolami and Calderhead (2011) aim at computing the *a posteriori* distribution of a statistical model of interest and thus choose $g$ to be the Fisher-Rao metric. However, this metric becomes untractable for models with high complexity. Therefore, Cobb et al. (2019) rather consider an empirical version of $g$ and combine it with the Soft-Abs method introduced by Betancourt (2013) to properly define a metric while preserving the statistical information.

In this paper, we consider another approach which exploits the geometrical structure of $M$, and does not rely on a given statistical framework. For instance, one can always define a self-concordant barrier $\phi$ when $M$ is a convex body, as explained by Nesterov and Nemirovskii (1994), and choose $g = D^2\phi$. This idea is also followed by Kook et al. (2022), whose aim is to sample from a Gibbs distribution over a convex bounded manifold of the form $M = \{x \in \mathbb{R}^d : Ax = b, \ell < x < u\}$. In contrast to our work, they do not perform a “reverse integration check”, and therefore cannot control the asymptotic bias of their method, see Section 7.

**Theoretical guarantees for RMHMC.** Elaborating on Riemannian geodesics, Lee and Vempala (2018) provide theoretical guarantees of fast mixing time for RMHMC when (i) $M$ is a polytope, and (ii) $g$ is the Hessian of a self-concordant function $\phi$ (as in our setting). Their result notably improves the complexity of uniform polytope sampling from algorithms relying on self-concordance such as the Dikin Walk (Kannan and Narayanan, 2009) and the Geodesic Walk (Lee and Vempala, 2017a). Crucially, they assume that the Hamiltonian dynamics can be exactly computed, which is not the case in practice. Proving the reversibility of practical implementations of RMHMC requires to control the numerical integrator used to approximate the Hamiltonian dynamics.

Zappa et al. (2018) propose a version of RWMH including projection steps after each proposal. To our knowledge, they are the first to check whether the “reverse integration” of the proposal is possible, and thus enforce the reversibility of the Markov chain with respect to $\pi$. Lelièvre et al. (2019) notably combine this method with the discretization suggested by Brubaker et al. (2012) to also enforce the constraints of the manifold. Lelièvre et al. (2022) elaborate on this framework, by designing a symplectic numerical integrator with multiple possible outputs, and provide a rigorous proof of reversibility. Note that it only applies when $g$ is induced by the flat metric of $\mathbb{R}^d$ and therefore cannot be combined with our approach as such. We leave the study of the extension of our work to this setting for future work.

7  Numerical experiments

In our experiments, we study the influence of the “reverse integration check” on the asymptotic bias and discuss the practical implications of the choice of the norm in (5) in a low two-dimensional setting. Then, we highlight that our algorithm can be adapted to handle constraints of the form $\{x \in \mathbb{R}^d : Ax < b, Bx = c\}$ and illustrate this by sampling from the uniform measure on the Birkhoff polytope.

In all of our settings, we sample the step-size at each iteration from the uniform distribution on $(0, h)$, where $h$ is a hyperparameter, as we observed that this choice allows for better exploration of the target measure. At each iteration, we perform one step of numerical integration, using the Störmer-Verlet scheme, using $K = 10$ fixed-point steps. We keep the refresh parameter to $\beta = 1$, and perform a thinning of the Markov chains by a factor 100. We refer to Appendix I for an ablation study of these parameters.

**Relevance of the reverse integration check.** We first compare n-BHMC with a version of itself which does not comprise the “reverse integration check” (i.e., $\eta = +\infty$). The obtained algorithm is then similar to the one of Kook et al. (2022). In order to correctly assess the bias of each method in a controlled setting, we consider the problem of accurately computing $\int_M f(x_1, x_2)\,dx_1\,dx_2$ on the hypercube $M = [-1, 1]^2$. We choose $f(x_1, x_2) = x_1^2$, referred to as square, and $f(x_1, x_2) = \cos(\pi x_2/2)$, referred to as cosine. In implementing n-BHMC, we observed that our method is sensitive to the value of the threshold $\eta$, and thus set $\eta = 10^{-i}$ for $i \in \{2, 3, 4, 5\}$. In Tables 1 and 2, we show that without any “reverse integration check”, the estimated quantities are biased. Adding this check improves the estimation and the lower the tolerance, the smaller the bias. However, a smaller $\eta$ hurts the mixing time of the algorithm as we reject more samples, as shown in Figure 3.

Following Lelièvre et al. (2022), we denote by FSR (Forward Success Rate) and BSR (Backward Success Rate) in Tables 1 and 2 the average success rate of check (a) and check (b) in the “reverse integration check” of n-BHMC (see Section 4.2) conditionally to success of check (a). Numbers are bold if the true value (1/3 for square and 2/π for cosine) is in the confidence interval given by the MCMC estimator.

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2Code soon available on GitHub.
Table 1: Results for $h = 0.3$ after 800k iterations of n-BHMC (average over 3 runs).

| Tolerance $\eta$ | square | cosine | FSR | BSR |
|------------------|--------|--------|-----|-----|
| $\eta = +\infty$ | $0.351 \pm 0.005$ | $0.619 \pm 0.005$ | 0.99 | 1.00 |
| $\eta = 10^{-4}$ | $0.332 \pm 0.014$ | $0.638 \pm 0.013$ | 0.99 | 0.95 |
| $\eta = 10^{-5}$ | $0.331 \pm 0.011$ | $0.638 \pm 0.011$ | 0.99 | 0.90 |

Table 2: Results for $h = 0.8$ after 800k iterations of n-BHMC (average over 3 runs).

| Tolerance $\eta$ | square | cosine | FSR | BSR |
|------------------|--------|--------|-----|-----|
| $\eta = +\infty$ | $0.312 \pm 0.002$ | $0.659 \pm 0.002$ | 0.94 | 1.00 |
| $\eta = 10^{-2}$ | $0.332 \pm 0.006$ | $0.638 \pm 0.006$ | 0.92 | 0.87 |
| $\eta = 10^{-3}$ | $0.323 \pm 0.009$ | $0.647 \pm 0.008$ | 0.93 | 0.77 |

This changes the problem of sampling on the space $\mathbb{R}^d$ in a problem of sampling on the space $\text{Ker}(B)$ and the solutions are reconstructed using $u \mapsto B^\dagger c + u$. Using this approach, we sample the uniform distribution on the Birkhoff polytope $M = \{ P \in [0,1]^{n \times n} : \sum_{i=1}^n P_{i,j} = 1, \sum_{j=1}^n P_{i,j} = 1, i,j \in [n] \}$, see Figure 5 (note that the dimension of $M$ is $d = (n-1)^2$).

Figure 5: Samples obtained with n-BHMC ($h = 0.3$ and $\eta = 10^{-2}$) at iteration 1000 and 3000.

We assess the convergence of our algorithm by showing that its moving average converges to the mean of the uniform distribution on $M$, see Figure 6. We emphasize, that without the "reverse integration check", the algorithm is unstable and degenerates near the boundary of $M$. While this degeneracy could be avoided by a careful adaptive choice of $h$ (Kook et al., 2022), the "reverse integration check" provides this stability as a by-product.

Figure 6: Frobenius norm between the true mean and its MCMC estimator for 100k iterations of n-BHMC (average over 3 runs), $h = 0.3$, $\eta = 10^{-2}$.

8 Discussion

In this paper, we introduced a novel version of RMHMC, Barrier HMC (BHMC), which addresses the problem of sampling a distribution $\pi$ over a constrained convex subset $M \subset \mathbb{R}^d$ equipped with a self-concordant barrier $\phi$. In particular, we propose two versions of BHMC, for which we prove that $\pi$ is invariant: (i) c-BHMC, where we assume that the Hamiltonian dynamics can be exactly computed, and (ii) n-BHMC, which is implemented in practice using approximations of this dynamics and a "reverse integration check". Under reasonable assumptions, our theory shows that the check performed in n-BHMC removes the asymptotic bias. This result is supported by numerical experiments highlighting this bias. In future work, we would like to investigate the "coupled" behaviour of the hyperparameters $h$ and $\eta$ in practice. Another promising extension is the study of irreductibility of n-BHMC and the influence of $\eta$ on the bias. Finally, we are interested in the application of n-BHMC for efficient polytope volume computation.
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Barrier Hamiltonian Monte Carlo

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Supplementary Material: Barrier Hamiltonian Monte Carlo

Organisation of the supplementary

This appendix is organized as follows. Appendix A summarizes general facts that will be useful for proofs. Appendix B and Appendix C provide additional details on Riemannian metrics and technicalities on self-concordance, respectively. Proofs of results on c-BHMC, that are stated in Section 3, are given in Appendix D. Appendix E presents general facts about numerical integration and specific facts on the integrators used in n-BHMC. Appendix F dispenses the proof of the result on implicit integrators of n-BHMC, stated in Section 5.1. Appendix G presents the modified version of n-BHMC, incorporating a step-size condition, for which we state the reversibility with respect to the target distribution in Section 5.2. Proof of this last result is given in Appendix H. Finally, Appendix I provides more details on the experiments of Section 7, as well as additional numerical results.

Notation. For any Riemannian manifold $(M, g)$ and any $z = (x, p) \in T^*M$, we denote by $\| \cdot \|_z$ the norm defined on $T^*M$ by $\|(x', p')\|_z = \|x'\|_{g(z)} + \|p'\|_{g(z)^{-1}}$ for any $(x', p') \in T^*M$. For any open subset $U \subset \mathbb{R}^d$ and any $k \in \mathbb{N}$, we denote by $C^k(U, \mathbb{R}^d)$ the set of functions $f : U \to \mathbb{R}^d$ such that $f$ is $k$ times continuously differentiable.

A Useful facts and lemmas

We recall here some basic knowledge on linear algebra and probability, and state useful inequalities for our proofs.

Linear algebra reminders. For any matrices $A, B \in \mathbb{R}^{d \times d}$, we write $A \preceq B$ if for any $x \in \mathbb{R}^d$, $x^T(B - A)x \geq 0$. Any positive-definite matrix $A \in \mathbb{R}^{d \times d}$ induces a scalar product $\langle \cdot, \cdot \rangle_A$ on $\mathbb{R}^d$, defined by $\langle x, y \rangle_A = (x, Ay)$. This scalar product induces the norm $\| \cdot \|_A$ on $\mathbb{R}^d$, defined by $\|x\|_A = \sqrt{x^T x} = \|A^{1/2}x\|_2$. For any positive-definite matrices $A, B \in \mathbb{R}^{d \times d}$ and for any $\alpha \geq 0$, $A \preceq \alpha B$ is equivalent to $\| \cdot \|_A \leq \sqrt{\alpha} \| \cdot \|_B$. The canonical norm of $\mathbb{R}^d$ induces the norm $\| \cdot \|_2$ on $\mathbb{R}^{d \times d}$, defined by $\|A\|_2 = \sup_{\|x\|_2 = 1} \|Ax\|_2$. In particular, for any matrices $A, B \in \mathbb{R}^{d \times d}$ and any vector $x \in \mathbb{R}^d$, $\|Ax\|_2 \leq \|A\|_2 \|x\|_2$ and $\|AB\|_2 \leq \|A\|_2 \|B\|_2$. Moreover, if $A$ is non-negative-definite, then $\|A\|_2 = \lambda(A)$, where $\lambda(A)$ is the largest eigenvalue of $A$, and $\|A^\alpha\|_2 = \lambda(A)^\alpha$ for any $\alpha > 0$.

Probability reminders. In this section, we consider a smooth manifold $M \subset \mathbb{R}^d$. We first recall the definition of reversibility (Douc et al., 2018, Definition 1.5.1) before stating general results on reversibility.

Definition 7. Let $Q : T^*M \times \mathcal{B}(T^*M) \to [0, 1]$ be a transition probability kernel and let $\bar{\pi}$ be a probability distribution on $T^*M$. Then,

(a) $Q$ is said to be reversible with respect to $\bar{\pi}$ if for any $f \in C(T^*M \times T^*M, \mathbb{R})$ with compact support

\[ \int_{T^*M \times T^*M} f(z, z') Q(z, dz') \bar{\pi}(dz) = \int_{T^*M \times T^*M} f(z', z) Q(z, dz') \bar{\pi}(dz). \]

(b) $Q$ is said to be reversible up to momentum reversal with respect to $\bar{\pi}$ if for any $f \in C(T^*M \times T^*M, \mathbb{R})$ with compact support

\[ \int_{T^*M \times T^*M} f(z, z') Q(z, dz') \bar{\pi}(dz) = \int_{T^*M \times T^*M} f(s(z'), s(z)) Q(z, dz') \bar{\pi}(dz), \]

where we recall that for any $(x, p) \in \mathbb{R}^d \times \mathbb{R}^d$, $s(x, p) = (x, -p)$.

Lemma 8. Let $Q : T^*M \times \mathcal{B}(T^*M) \to [0, 1]$ be a transition probability kernel and let $\bar{\pi}$ be a probability distribution on $T^*M$. Assume that $s_{xy} \bar{\pi} = \bar{\pi}$ and that $Q$ is reversible up to momentum reversal with respect to $\bar{\pi}$. Then $\bar{\pi}$ is an invariant measure for $Q$, i.e., for any $f \in C(T^*M, \mathbb{R})$ with compact support

\[ \int_{T^*M \times T^*M} f(z') Q(z, dz') \bar{\pi}(dz) = \int_{T^*M \times T^*M} f(z) \bar{\pi}(dz). \]
Proof. Let $f \in C(T^*M, \mathbb{R})$ with compact support. We have
\[
\int_{T^*M} f(z')Q(z, dz')\bar{\pi}(dz) = \int_{T^*M} f(z)Q(s(z), dz')\bar{\pi}(dz) \quad \text{(Definition 7)}
\]
and
\[
= \int_{T^*M} f(z)Q(s(z), dz')\bar{\pi}(dz) = \int_{T^*M} f(z)\bar{\pi}(dz) \quad \text{(momentum reversal on $z$)}
\]
which concludes the proof.

Lemma 9. Let $Q : T^*M \times \mathcal{B}(T^*M) \to [0, 1]$ be a transition probability kernel and let $\bar{\pi}$ be a probability distribution on $T^*M$. Assume that $s\#Q = Q$ and that $Q$ is reversible with respect to $\bar{\pi}$. Then, $Q$ is reversible up to momentum reversal with respect to $\bar{\pi}$.

Proof. Let $f \in C(T^*M, \mathbb{R})$ with compact support. We have
\[
\int_{T^*M} f(z', z')Q(z, dz')\bar{\pi}(dz) = \int_{T^*M} f(z, s(z'))Q(z, dz')\bar{\pi}(dz) \quad \text{(momentum reversal on $z'$)}
\]
and
\[
= \int_{T^*M} f(z', s(z))Q(z, dz')\bar{\pi}(dz) = \int_{T^*M} f(z', s(z))\bar{\pi}(dz) \quad \text{(Definition 7)}
\]
and
\[
= \int_{T^*M} f(s(z'), s(z))Q(z, dz')\bar{\pi}(dz) = \int_{T^*M} f(s(z'), s(z))\bar{\pi}(dz) \quad \text{(momentum reversal on $z'$)}
\]
which concludes the proof.

Useful inequalities. The following inequalities hold: (a) for any $u \in [0, 1/5], (1 - u)^{-2} \leq 1 + 3u$ and $(1 - u)^{-3} \leq 1 + 5u$, (b) for any $u \in [0, 1/2], (1 - u)^{-1} \leq 1 + 2u$, (c) for any $u \in [0, 1], (1 - u)^{2} - 1 \leq 3u$, (d) for any $u \geq 0$, we have $1 - (1 + u)^{-1} \leq u$ and $(1 - u)^{2} - 1 \geq -2u$.

B Details on Riemannian metrics

Let $M$ be a smooth $d$-dimensional manifold, endowed with a metric $g$. We recall that the Riemannian volume element corresponding to $(M, g)$ is given in local coordinates by $d\text{vol}_M(x) = \sqrt{|\det(g)|}dx$, where $dx$ is a coframe, (Lee, 2006, Lemma 3.2.). For any $x \in M$, we respectively denote by $T_xM$ and $T_x^*M$, the tangent space at $x$ and its dual space, i.e., the cotangent space at $x$. Note that $T_xM$ and $T_x^*M$ are space vectors, and $T_x^*M$ is endowed with the scalar product $\langle \cdot, \cdot \rangle_{g(x)}$ by definition of the Riemannian metric. For clarity sake, we denote by $v$ (resp. $p$) an element of the tangent (resp. cotangent) space. We recall that the tangent bundle $TM$ and the cotangent bundle $T^*M$ are respectively defined by $TM = \bigsqcup_{x \in M}\{x\} \cup T_xM$ and $T^*M = \bigsqcup_{x \in M}\{x\} \cup T_x^*M$ and $\{x\}$ is endowed with the scalar product $\langle \cdot, \cdot \rangle_{g(x)}$ by definition of the Riemannian metric. For clarity sake, we denote by $v$ (resp. $p$) an element of the tangent (resp. cotangent) space. We recall that the tangent bundle $TM$ and the cotangent bundle $T^*M$ are respectively defined by $TM = \bigsqcup_{x \in M}\{x\} \cup T_xM$ and $T^*M = \bigsqcup_{x \in M}\{x\} \cup T_x^*M$ and $\{x\}$ is endowed with the scalar product $\langle \cdot, \cdot \rangle_{g(x)}$ by definition of the Riemannian metric.

Metric on the tangent bundle $TM$. Sasaki (1958) originally introduced on $TM$ a Riemannian metric $\hat{g}$, which, among other properties, preserves the Euclidean metric induced by $g$ on each tangent space. This metric is defined by
\[
\hat{g} = \left( g_{ij} + v^k v^{\ell}_i \Gamma^i_{k \ell} g_{st} - g^{is} v^k \Gamma^k_{js} \right)
\]
where $g_{ij}$ and $g^{ij}$ respectively refer to $g$ and $g^{-1}$, and $\Gamma$ corresponds to the Christoffel symbol. Since $(TM, \hat{g})$ is a Riemannian manifold, the volume form on $TM$ satisfies for any $(x, v) \in TM$
\[
d\text{vol}_{TM}(x, v) = \sqrt{\det(\hat{g}(x, v))}dx = \det(g(x, v))dx .
\]

Metric on the cotangent bundle $T^*M$. Elaborating on the metric defined by Sasaki (1958), Mok (1977) showed that for any $x \in M, T_x^*M$ is naturally endowed with the scalar product $\langle \cdot, \cdot \rangle_{g(x)}^{-1}$, and proposed a Riemannian metric $g^*$ on $T^*M$, which notably preserves this result on each cotangent space. This metric is closely related to $\hat{g}$ and is defined by
\[
g^* = \left( g_{ij} + p^k p^{\ell}_i \Gamma^i_{k \ell} g_{st} - g^{is} p^k \Gamma^k_{js} \right)
\]
Since $(T^*M, g^*)$ is a Riemannian manifold, the volume form on $T^*M$ satisfies for any $(x, p) \in T^*M$
\[
d\text{vol}_{T^*M}(x, p) = \sqrt{\det(g^*(x, p))}dx = dx dp .
\]
In contrast to the tangent bundle, the volume form on the cotangent bundle does not depend on $g$, which motivates to augment on $T^*M$ (instead of $TM$) any target measure $\pi$ defined on $M$. 

C Properties of self-concordance

We first recall the definition of self-concordance and derive some of its properties in Lemmas 11 and 12.

**Definition 10 (Nesterov and Nemirovskii (1994)).** Let $U$ be a non-empty open convex domain in $\mathbb{R}^d$. A function $\phi : U \to \mathbb{R}$ is said to be a $\nu$-self-concordant barrier (with $\nu \geq 1$) on $U$ if it satisfies:

(a) $\phi \in C^3(U, \mathbb{R})$ and $\phi$ is convex,
(b) $\phi(x) \to +\infty$ as $x \to \partial U$,
(c) $|D^3\phi(x)[h, h, h]| \leq 2\|h\|_{\phi(x)}^2$, for any $x \in M$, $h \in \mathbb{R}^d$,
(d) $|D\phi(x)[h]|^2 \leq \nu\|h\|_{\phi(x)}^2$, for any $x \in M$, $h \in \mathbb{R}^d$,

where $g(x) = D^2\phi(x)$.

Self-concordance can be thought as a certain kind of regularity. Indeed, if $\phi$ is a $\nu$-self-concordant barrier on a convex body $U$, then $D^2\phi$ is $2$-Lipschitz continuous on $U$ with respect to the local norm induced by $g$ (see Property (c)), and more restrictively, $\phi$ is $\nu$-Lipschitz continuous with respect to the same norm (see Property (d)).

**Lemma 11.** Let $\phi : U \to \mathbb{R}$ be a $\nu$-self-concordant barrier with $g = D^2\phi$. Assume that $U$ is bounded. Then, $\|\nabla\phi(x)\|_2 \to +\infty$ and $\|g(x)\|_2 \to +\infty$ as $x \to \partial U$.

**Proof.** Since $\phi$ is convex, we have, for any $(x, y) \in U^2$

$$\phi(x) \leq \phi(y) + \nabla \phi(x)(x - y),$$

$$|\phi(x)| \leq |\phi(y)| + \|\nabla \phi(x)\|_2 \|x - y\|_2$$

$$\leq |\phi(y)| + \|\nabla \phi(x)\|_2 \text{diam}(U),$$

where we used Cauchy-Schwartz inequality in the second line. Using Property (b) of $\phi$, we obtain that $\|\nabla\phi(x)\|_2 \to +\infty$ as $x \to \partial U$. By combining this result with Property (d) of $\phi$, we obtain that $\|g(x)\|_2 \to +\infty$ as $x \to \partial U$.

According to Nesterov (2003) (see Lemma 4.1.2), Property (c) of self-concordance is equivalent to

$$|D^3\phi(x)[h_1, h_2, h_3]| \leq 2\prod_{i=1}^3 \|h_i\|_{\phi(x)},$$

for any $x \in M$ and any $(h_1, h_2, h_3) \in \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d$.

Let $u : \mathbb{R}^d \to \mathbb{R}^d$ be a linear operator. For any $x \in \mathbb{R}^d$, we define the operator norms $\|u\|_{\phi(x)}$ and $\|u\|_{\phi(x)^{-1}}$ by

$$\|u\|_{\phi(x)} = \sup\{u(g(x)h) : \|h\|_{\phi(x)} = 1\},$$

$$\|u\|_{\phi(x)^{-1}} = \sup\{u(g(x)^{-1}h) : \|h\|_{\phi(x)^{-1}} = 1\}.$$

In addition, a set $V \subset \mathbb{R}^d$ contains no straight line if for any $D_{x_0} = \{tx_0 : t \in \mathbb{R}\}$ with $x_0 \neq 0$, we have $V^c \cap D_{x_0} \neq \emptyset$.

**Lemma 12.** Let $\phi : U \to \mathbb{R}$ be a $\nu$-self-concordant barrier with $g = D^2\phi$. Assume that $U$ contains no straight line. For any $x \in U$ and any $r > 0$, we denote by $W^0(x, r)$ the open Dikin ellipsoid of $\phi$ at $x$, given by $W^0(x, r) = \{y \in \mathbb{R}^d | \|y - x\|_{\phi(x)} < r\}$. Then, the following properties hold:

(a) For any $x \in U$ and any $(h_1, h_2) \in \mathbb{R}^d \times \mathbb{R}^d$

$$\|D^3\phi(x)[h_1, h_2]\|_{\phi(x)^{-1}} \leq 2\|h_1\|_{\phi(x)}\|h_2\|_{\phi(x)}.$$

(b) For any $x \in U$, $W^0(x, 1) \subset U$, and for any $y \in W^0(x, 1)$

$$\left(1 - \|y - x\|_{\phi(x)}\right)^2 g(x) \leq g(y) \leq \left(1 - \|y - x\|_{\phi(x)}\right)^{-2} g(x).$$

(c) For any $x \in U$, any $y \in W^0(x, 1)$ and any $h \in \mathbb{R}^d$, the following hold

$$\|h\|_{\phi(x)} \leq \left(1 - \|y - x\|_{\phi(x)}\right)^{-1} \|h\|_{\phi(y)} ,$$

$$\|h\|_{\phi(y)} \leq \left(1 - \|y - x\|_{\phi(x)}\right)^{-1} \|h\|_{\phi(x)} ,$$

$$\|h\|_{\phi(x)^{-1}} \leq \left(1 - \|y - x\|_{\phi(x)}\right)^{-1} \|h\|_{\phi(y)^{-1}} ,$$

$$\|h\|_{\phi(y)^{-1}} \leq \left(1 - \|y - x\|_{\phi(x)}\right)^{-1} \|h\|_{\phi(x)^{-1}} .$$
Proof. The result is a direct consequence of (Nesterov, 2003, Theorem 4.1.3, Theorem 4.1.5, Theorem 4.1.6).

We now introduce $\alpha$-regularity, which slightly strengthens self-concordance, by ensuring that $D^3\phi$ is $\alpha(\alpha + 1)$-Lipschitz continuous with respect to the local norm induced by $g$ (see (7)). We state below the definition of $\alpha$-regularity as well as some of its properties in Lemma 14.

**Definition 13** (Nesterov and Nemirovskii (1998)). Let $\alpha \geq 1$ and $U$ be non-empty open convex domain in $\mathbb{R}^d$. A self-concordant function $\phi$ on $U$ is said $\alpha$-regular, if $\phi \in C^4(U, \mathbb{R})$ and for any $x \in U$ and any $h \in \mathbb{R}^d$

$$|D^4\phi(x)[h, h, h, h]| \leq \alpha(\alpha + 1)\|h\|_{g(x)}^2 \|h\|_{U,x}^2,$$

where $\|h\|_{U,x} := \inf \{t^{-1} \mid t > 0, x \pm th \in U\}$.

**Lemma 14.** Let $\phi : U \to \mathbb{R}$ be a $\alpha$-regular function with $g = D^2\phi$. Assume that $U$ contains no straight line.

(a) For any $x \in U$ and any $h \in \mathbb{R}^d$

$$|D^4\phi(x)[h, h, h, h]| \leq \alpha(\alpha + 1)\|h\|_{g(x)}^4.$$

(b) For any $x \in U$, any $(h_1, h_2, h_3, h_4) \in \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d$

$$|D^4\phi(x)[h_1, h_2, h_3, h_4]| \leq \alpha(\alpha + 1)\prod_{i=1}^4 \|h_i\|_{g(x)}.$$

(c) For any $x \in U$, any $y \in W^0(x, 1)$ and any $(h_1, h_2) \in \mathbb{R}^d \times \mathbb{R}^d$

$$|D^3\phi(x)[h_1, h_2] - D^3\phi(y)[h_1, h_2]|_{g(x)} \leq \frac{\alpha(\alpha + 1)}{3}\|h_1\|_{g(x)}\|h_2\|_{g(x)}((1 - \|y - x\|_{g(x)})^{-3} - 1).$$

**Proof.** We first prove (7). First remark that the result is true for $h = 0$. Consider now $h \neq 0$. Let $\varepsilon > 0$. We define $t_\varepsilon = (1 + \varepsilon)^{-1}\|h\|_{g(x)}^{-1} > 0$, $y_\varepsilon^+ = x + t_\varepsilon h$ and $y_\varepsilon^- = x - t_\varepsilon h$. We have $\|x - y_\varepsilon^-\|_{g(x)} = \|x - y_\varepsilon^+\|_{g(x)} = 1/(1 + \varepsilon) < 1$. Hence, $y_\varepsilon^+ \in U$ and $y_\varepsilon^- \in U$ by Lemma 12. Therefore, $\|h\|_{U,x} \leq t_\varepsilon^{-1}$ and

$$|D^4\phi(x)[h, h, h, h]| \leq \alpha(\alpha + 1)\|h\|_{g(x)}^4(1 + \varepsilon)^2.$$

We conclude upon taking $\varepsilon \to 0$. Then, (8) is an immediate consequence of (7) using (Nesterov and Nemirovskii, 1994, Proposition 9.1.1). We now prove (9). Using Lemma 12, we have

$$\|D^3\phi(x)[h_1, h_2] - D^3\phi(y)[h_1, h_2]|_{g(x)}^{-1} \leq \int_0^1 \|D^3\phi(x + t(y - x))[h_1, h_2, y - x]|_{g(x)}^{-1} dt$$

$$\leq \int_0^1 (1 - t)\|y - x\|_{g(x)}^{-1} |D^4\phi(x + t(y - x))[h_1, h_2, y - x]|_{g(x)}^{-1} dt$$

$$\leq \alpha(\alpha + 1)/(1 - t)\|y - x\|_{g(x)}(1 - t)\|y - x\|_{g(x)}^{-1}$$

$$\leq \alpha(\alpha + 1)/3\|h_1\|_{g(x)}\|h_2\|_{g(x)}\int_0^1 |y - x\|_{g(x)}/(1 - t)\|y - x\|_{g(x)} dt$$

which concludes the proof.

We now prove the equivalence between the Euclidean norm and the norms induced by $g$ and $g^{-1}$.

**Lemma 15.** Let $(U, g)$ be non-empty Riemannian manifold in $\mathbb{R}^d$. For any $x_0 \in U$, any $(x, p) \in U \times \mathbb{R}^d$, we have

$$\|g(x_0)^{-1}\|^{-1/2}_2 \|x\|_2 \leq \|x\|_{g(x_0)} \leq \|g(x_0)\|^{1/2}_2 \|x\|_2,$$

$$\|g(x_0)^{-1}\|^{-1/2}_2 \|p\|_2 \leq \|p\|_{g(x_0)^{-1}} \leq \|g(x_0)^{-1}\|^{1/2}_2 \|p\|_2.$$

In addition, let

$$C_{x_0} = \max(\|g(x_0)\|^{1/2}_2, \|g(x_0)^{-1}\|^{1/2}_2) > 0.$$

Then, we have

$$1/C_{x_0}(\|x\|_2 + \|p\|_2) \leq \|x\|_{g(x_0)} + \|p\|_{g(x_0)^{-1}} \leq C_{x_0}(\|x\|_2 + \|p\|_2).$$
D  Proofs of Section 3

D.1  Existence, uniqueness and explosion time of Hamiltonian dynamics

We prove below Proposition 2 and Proposition 3.

Proof of Proposition 2. Assume A1, A2. In particular, M contains no straight line, and Lemmas 12 and 14 apply here. We rewrite the ODE (3) as a Cauchy problem defined on Banach space $E = (\mathbb{R}^d \times \mathbb{R}^d, \| \cdot \|_E)$ where $\|(a, b)\|_E = \|a\|_2 + \|b\|_2$ for any pair $(a, b) \in \mathbb{R}^d \times \mathbb{R}^d$. We define $\Omega = M \times \mathbb{R}^d$, which is an open set in $E$. A solution $(J, z)$ to this Cauchy problem is defined for all $t \in J$ by

$$
\dot{z}(t) = F(z(t)), \quad z(0) = z_0, \quad \text{where} \quad F(x, p) = (\partial_p H(x, p), -\partial_x H(x, p)),
$$

such that $J$ is an open interval of $\mathbb{R}$ with $0 \in J$, and $z = (x, p) : J \to \Omega$ is differentiable on $J$. We now prove two results on $F$ to establish existence and uniqueness of a maximal solution $(J, z)$ for this Cauchy problem:

(a) $F$ is continuously differentiable on $\Omega$.

(b) $F$ is locally Lipschitz-continuous on $\Omega$ with respect to $\| \cdot \|_E$.

Since $\nabla V, Dg \in C^1(M, \mathbb{R})$, we directly obtain Item (a). We now prove Item (b). Let $\bar{z} = (\bar{x}, \bar{p}) \in \Omega$. We endow $E$ with the norm $\| \cdot \|_{\bar{z}}$. Since $M$ is an open subset of $\mathbb{R}^d$, there exists $0 < r \leq 1/(11C_E)$, where we recall that $C_E$ is defined in Lemma 15, such that $B_{\| \cdot \|_{\bar{z}}} (\bar{x}, r) \subset M$. We consider such $r$, and we define $B = B_{\| \cdot \|_{\bar{z}}} (\bar{x}, r)$ and $B_g = B_{\| g \cdot \|_{\bar{z}}} (\bar{x}, \bar{r})$, where $\bar{r} = C_2 r \leq 1/11$. In particular, we have by Lemma 12-(b) that $B_g \subset B_{\| g \cdot \|_{\bar{x}}}(\bar{x}, \bar{r}) \times B_{\| g \cdot \|_{\bar{x}}}(\bar{x}, \bar{r}) \subset \Omega$ since $\bar{r} < 1$. Moreover, using Lemma 15, we have $B \subset B_g \subset \Omega$.

Since $V \in C^2(M, \mathbb{R})$, $\nabla V$ is Lipschitz-continuous on $B_g$, i.e., there exists $C_V > 0$ such that for any $(z, z') \in B_g \times B_g$,

$$
\| \nabla V(x) - \nabla V(x') \|_{\bar{z}} \leq C_V \| x - x' \|_{\bar{z}},
$$

We now show that $F$ is Lipschitz-continuous on $B_g$ with respect to $\| \cdot \|_{\bar{z}}$.

Consider $(z, z') \in B_g \times B_g$ denoted by $z = (x, p)$ and $z' = (x', p')$. Note that $(x, x') \in W^0(\bar{x}, 1) \times W^0(\bar{x}, 1)$, where $W^0(\bar{x}, 1)$ is defined in Lemma 12. We first bound $\|F(1)(z) - F(1)(z')\|_{\bar{z}} = \|\partial_p H(z) - \partial_p H(z')\|_{\bar{z}}$. We have

$$
\partial_p H(z) - \partial_p H(z') = g(x)^{-1}p - g(x')^{-1}p' = g(x)^{-1}(p - p') + (g(x)^{-1} - g(x')^{-1})p',
$$

then,

$$
\|\partial_p H(z) - \partial_p H(z')\|_{\bar{z}} \leq \|g(x)^{1/2}g(x)^{-1}g(x)^{1/2}\|_2 \|p - p'\|_{\bar{z}} + \|g(x)^{1/2}g(x)^{-1} - g(x')^{-1}\|g(x)^{1/2}\|_2 \|p'\|_{\bar{z}}. \tag{11}
$$

Using Lemma 12-(b), we have

$$
(1 - \|\bar{x} - x\|_{\bar{z}})^2 g(\bar{x})^{-1} \leq g(x)^{-1} \leq (1 - \|\bar{x} - x\|_{\bar{z}})^{-2} g(\bar{x})^{-1},
$$

and thus,

$$
(1 - \|\bar{x} - x\|_{\bar{z}})^2 1_d \leq g(\bar{x})^{1/2} g(x)^{-1} g(\bar{x})^{1/2} \leq (1 - \|\bar{x} - x\|_{\bar{z}})^{-2} 1_d
$$

and therefore,

$$
(1 - \bar{r})^2 1_d \leq g(\bar{x})^{1/2} g(x)^{-1} g(\bar{x})^{1/2} \leq (1 - \bar{r})^{-2} 1_d.
$$

Therefore, we have

$$
\|g(\bar{x})^{1/2} g(x)^{-1} g(\bar{x})^{1/2}\|_2 \leq (1 - \bar{r})^{-2}. \tag{12}
$$

In addition, we have

$$
\|x - x'\|_{\bar{z}} \leq (1 - \|\bar{x} - x'\|_{\bar{z}})^{-1} \|x - x\|_{\bar{z}} < (1 - \bar{r})^{-1} 2\bar{r} < 1/5. \tag{13}
$$
where we used Lemma 12-(c) in the first inequality and \( \bar{r} \leq 1/11 \) in the last inequality.

Therefore, \( x' \in \mathcal{W}^0(x,1) \) and we have using Lemma 12-(b)
\[
\begin{align*}
\{(1 - \|x' - x\|_{\bar{g}(x)}^2 - 1) \bar{g}(x')^{-1} & \leq \bar{g}(x)^{-1} - \bar{g}(x')^{-1} \\
\{(1 - \|x' - x\|_{\bar{g}(x)}^2 - 1) \bar{I}_d & \leq \bar{g}(x)^{1/2}(\bar{g}(x)^{-1} - \bar{g}(x')^{-1})\bar{g}(x)^{1/2} \leq \{(1 - \|x' - x\|_{\bar{g}(x)}^2 - 1) (1 - \bar{r})^{-2}\bar{I}_d .
\end{align*}
\]

Then,
\[
\|\bar{g}(x)^{1/2}(\bar{g}(x)^{-1} - \bar{g}(x')^{-1})\bar{g}(x)^{1/2}\|_2 \leq \max\{(1 - \|x' - x\|_{\bar{g}(x)}^2 - 1)(1 - \bar{r})^2, \{(1 - \|x' - x\|_{\bar{g}(x)}^2 - 1) (1 - \bar{r})^{-2}\}
\leq (1 - \bar{r})^{-2} \max\{(1 - \|x' - x\|_{\bar{g}(x)}^2 - 1), (1 - \|x' - x\|_{\bar{g}(x)}^2)^{-1} - 1\} .
\]

Using Inequalities (a) and (c) with \( u = \|x' - x\|_{\bar{g}(x)} \), where \( u \leq 1/5 \) by (13), we obtain
\[
\begin{align*}
(i) \quad (1 - \|x' - x\|_{\bar{g}(x)}^2 - 1) & \leq 3\|x' - x\|_{\bar{g}(x)} < 3(1 - \bar{r})^{-1}\|x - x'\|_{\bar{g}(x)} , \\
(ii) \quad (1 - \|x' - x\|_{\bar{g}(x)}^2 - 1) & \leq 3\|x' - x\|_{\bar{g}(x)} < 3(1 - \bar{r})^{-1}\|x - x'\|_{\bar{g}(x)} .
\end{align*}
\]

Moreover, we have
\[
\|p'\|_{\bar{g}(x)^{-1}} = \|p' - \bar{p} + \bar{p}\|_{\bar{g}(x)^{-1}} \leq \bar{r} + \|\bar{p}\|_{\bar{g}(x)^{-1}} .
\]

Combining (11), (12) and (14), it comes that
\[
\|F^{(1)}(z) - F^{(1)}(z')\|_{\bar{g}(x)} \leq (1 - \bar{r})^{-2}\|p - p'\|_{\bar{g}(x)^{-1}} + 3(1 - \bar{r})^{-3}(\bar{r} + \|\bar{p}\|_{\bar{g}(x)^{-1}})\|x - x'\|_{\bar{g}(x)} .
\]

We define \( A_{\bar{z},1} = (1 - \bar{r})^{-2} + 3(1 - \bar{r})^{-3}(\bar{r} + \|\bar{p}\|_{\bar{g}(x)^{-1}}) \), such that \( \|F^{(1)}(z) - F^{(1)}(z')\|_{\bar{g}(x)} \leq A_{\bar{z},1}\|z - z'\|_{\bar{z}} .
\]

We now bound \( \|F^{(2)}(z) - F^{(2)}(z')\|_{\bar{g}(x)^{-1}} = \|\partial_x H(z) - \partial_x H(z')\|_{\bar{g}(x)^{-1}} . \) We have
\[
\partial_x H(z) - \partial_x H(z') = \nabla V(x) - \nabla V'(x)
\]
\[
+ \frac{1}{2} Dg(x')[g(x')^{-1}p', g(x')^{-1}p'] - \frac{1}{2} Dg(x)[g(x)^{-1}p, g(x)^{-1}p]
\]
\[
+ \frac{1}{2} g(x)^{-1} : Dg(x) - \frac{1}{2} g(x')^{-1} : Dg(x')
\]

We have
\[
\|Dg(x')[g(x')^{-1}p', g(x')^{-1}p'] - Dg(x)[g(x)^{-1}p, g(x)^{-1}p]\|_{\bar{g}(x)^{-1}}
\]
\[
\leq \|Dg(x)[g(x)^{-1}p, g(x)^{-1}p] - Dg(x)[g(x')^{-1}p', g(x')^{-1}p']\|_{\bar{g}(x)^{-1}}
\]
\[
+ \|Dg(x)[g(x')^{-1}p', g(x')^{-1}p'] - Dg(x')[g(x')^{-1}p', g(x')^{-1}p']\|_{\bar{g}(x)^{-1}}
\]

Note that we have \( g(x)^{-1}p = F^{(1)}(z) \) (resp. \( g(x')^{-1}p' = F^{(1)}(z') \)). Using Lemma 12-(c), the first upper bound in (17) is bounded by
\[
(1 - \bar{r})^{-1}\|Dg(x)[F^{(1)}(z), F^{(1)}(z)] - Dg(x)[F^{(1)}(z'), F^{(1)}(z')]\|_{\bar{g}(x)^{-1}}
\]
\[
\leq 2(1 - \bar{r})^{-1}\|Dg(x)[F^{(1)}(z') - F^{(1)}(z)], F^{(1)}(z')]\|_{\bar{g}(x)^{-1}}
+ (1 - \bar{r})^{-1}\|Dg(x)[F^{(1)}(z') - F^{(1)}(z)], F^{(1)}(z') - F^{(1)}(z)]\|_{\bar{g}(x)^{-1}}
\leq 4(1 - \bar{r})^{-1}\|F^{(1)}(z') - F^{(1)}(z)]\|_{\bar{g}(x)^{-1}} + 2(1 - \bar{r})^{-1}\|F^{(1)}(z') - F^{(1)}(z)]\|_{\bar{g}(x)}^2 \quad \text{(Lemma 12-(a))}
\]
\[
\leq 4(1 - \bar{r})^{-3}\|F^{(1)}(z') - F^{(1)}(z)]\|_{\bar{g}(x)^{-1}} + 2(1 - \bar{r})^{-3}\|F^{(1)}(z') - F^{(1)}(z)]\|_{\bar{g}(x)}^2 \quad \text{(Lemma 12-(c))}
\]
\[
\leq 4(1 - \bar{r})^{-3}A_{\bar{z},1}\|z - z'\|_{\bar{z}} + 2(1 - \bar{r})^{-3}A_{\bar{z},1}\|z - z'\|_{\bar{z}}^2
\]
\[
\leq 4A_{\bar{z},1}(1 - \bar{r})^{-3}(\bar{r} + \|\bar{p}\|_{\bar{g}(x)^{-1}}) + 4(1 - \bar{r})^{-3}A_{\bar{z},1}\|z - z'\|_{\bar{z}} .
\]
where we used that $\|F^{(1)}(z')\|_{g(\bar{x})} \leq (1 - \bar{r})^{-2}(\bar{r} + \|\bar{p}\|_{g(\bar{x})^{-1}})$ in the last inequality. Combining Lemma 12(c) and Lemma 14(c), the second upper bound in (17) is bounded by

$$(1 - \bar{r})^{-1}||Dg(\bar{x})[F^{(1)}(z'), F^{(1)}(z')] - Dg(x')[F^{(1)}(z'), F^{(1)}(z')]||_{g(\bar{x})^{-1}}$$

\[ \leq \alpha(\alpha + 1)(1 - \bar{r})^{-1}/3 \{ (1 - \|x' - x\|_{g(\bar{x})}^{-3}) - 1 \} \|F^{(1)}(z')\|_{g(\bar{x})}^{2} \]

\[ \leq \alpha(\alpha + 1)(1 - \bar{r})^{-3}/3 \{ (1 - (1 - \bar{r})^{-1}\|x' - x\|_{g(\bar{x})}^{-3}) - 1 \} \|F^{(1)}(z')\|_{g(\bar{x})}^{2} \]

\[ \leq \alpha(\alpha + 1)(1 - \bar{r})^{-7}(\bar{r} + \|\bar{p}\|_{g(\bar{x})^{-1}})2/3 \{ (1 - (1 - \bar{r})^{-1}\|x' - x\|_{g(\bar{x})}^{-3}) - 1 \} . \]

Using Inequality (a) with $u = (1 - \bar{r})^{-1}\|x' - x\|_{g(\bar{x})}$, where $u \leq 1/5$ by (13), we obtain

$$(1 - (1 - \bar{r})^{-1}||x' - x||_{g(\bar{x})})^{-3} - 1 \leq 5(1 - \bar{r})^{-1}||x' - x||_{g(\bar{x})} . \tag{18}$$

Then, the second upper bound in (17) is bounded by

$$(5/3)\alpha(\alpha + 1)(1 - \bar{r})^{-8}(\bar{r} + \|\bar{p}\|_{g(\bar{x})^{-1}})^{2}||x' - x||_{g(\bar{x})} .$$

We now define $h : y \in M \rightarrow g(y)^{-1} : Dg(y)$. Since $\phi \in C^{1}(M), h \in C^{1}(M)$. Moreover, $[x, x'] \in M$ by convexity of $M$ and we can define $A_{\phi} = \sup_{y \in [x, x']} ||Dh(y)||$, where $||Dh(y)|| = \sup_{||u||_{g(\bar{x})} = 1} ||Dh(y)||$. Using the mean value theorem on $h$, we have

$$||h(x) - h(x')||_{g(\bar{x})^{-1}} \leq A_{\phi}||x' - x||_{g(\bar{x})} . \tag{19}$$

By combining (10), (16), (17) and (19), we have

$$||F^{(2)}(z) - F^{(2)}(z')||_{g(\bar{x})^{-1}} \leq C_{V}||x' - x||_{g(\bar{x})}$$

\[ + (1/2)\{ 4A_{\bar{x},1}(1 - \bar{r})^{-5}(\bar{r} + \|\bar{p}\|_{g(\bar{x})^{-1}}) + 4A_{\bar{x},1}(1 - \bar{r})^{-3}\bar{r} \} ||x' - x||_{g(\bar{x})} \]

\[ + (1/2) \cdot (5/3)\alpha(\alpha + 1)(1 - \bar{r})^{-8}(\bar{r} + \|\bar{p}\|_{g(\bar{x})^{-1}})^{2}||x' - x||_{g(\bar{x})} \]

\[ + (1/2)A_{\phi}||x' - x||_{g(\bar{x})} . \]

We define $A_{\bar{x},2} = C_{V} + 2A_{\bar{x},1}(1 - \bar{r})^{-5}(\bar{r} + \|\bar{p}\|_{g(\bar{x})^{-1}}) + 4A_{\bar{x},1}(1 - \bar{r})^{-3}\bar{r} + (5/6)\alpha(\alpha + 1)(1 - \bar{r})^{-8}(\bar{r} + \|\bar{p}\|_{g(\bar{x})^{-1}})^{2} + A_{\phi}/2$ such that

$$||F^{(2)}(z) - F^{(2)}(z')||_{g(\bar{x})} \leq A_{\bar{x},2}||z' - z||_{\bar{z}} .$$

Finally, we have

$$||F(z) - F(z')||_{\bar{z}} = ||F^{(1)}(z) - F^{(1)}(z')||_{g(\bar{x})} + ||F^{(2)}(z) - F^{(2)}(z')||_{g(\bar{x})^{-1}} \leq (A_{\bar{x},1} + A_{\bar{x},2})||z' - z||_{\bar{z}} ,$$

i.e., $F$ is $(A_{\bar{x},1} + A_{\bar{x},2})$-Lipschitz-continuous on $B_{\bar{g}}$ with respect to $\| \cdot \|_{\bar{z}}$.

We now show that $F$ is Lipschitz-continuous on $B$ with respect to $\| \cdot \|_{E}$.

Consider $(z, z') \in B \times B$ denoted by $z = (x, p)$ and $z' = (x', p')$. In particular, $(z, z') \in B_{\bar{g}} \times B_{\bar{g}}$. Using the previous result and Lemma 15, we have

$$||F(z) - F(z')||_{E} \leq C_{E}||F(z) - F(z')||_{\bar{z}} \leq C_{E}(A_{\bar{x},1} + A_{\bar{x},2})||z - z'||_{\bar{z}} \leq C_{E}^{2}(A_{\bar{x},1} + A_{\bar{x},2})||z - z'||_{E} ,$$

which proves that $F$ is $C_{E}^{2}(A_{\bar{x},1} + A_{\bar{x},2})$-Lipschitz-continuous on $B$ with respect to $\| \cdot \|_{E}$.

**Conclusion.** Combining Items (a) and (b), we obtain the results (i), (ii) and (iii) of Proposition 2 upon using Cauchy-Lipschitz’s theorem. Moreover, for any $t \in \mathcal{J}_{T_{\bar{z}}}, \partial_{t}H(z(t)) = \partial_{x}H(z(t))^{T} \dot{x}(t) + \partial_{p}H(z(t))^{T} \dot{p}(t) = -\dot{p}(t)^{T} \dot{x}(t) + \dot{p}(t)^{T} \dot{z}(t) = 0$, which proves the result (iv) of Proposition 2.

**Proof of Proposition 3.** Assume A1, A2. Let $z_{0} \in T^{*}M, (J_{z_{0}}, \bar{z})$ as in Proposition 2. Assume that $T_{z_{0}} = \sup J_{z_{0}} < +\infty$. Then, by Cauchy-Lipschitz’s theorem, $z$ leaves any compact set of $E$ at the neighbourhood of $T_{z_{0}}$. By construction of $\| \cdot \|_{E}$, this property is induced on both variables $x \in M$ and $p \in \mathbb{R}^{d}$, each with respect to $\| \cdot \|_{2}$. We directly obtain the result of Proposition 3 by continuity of $(x, p)$. □
D.2 Proof of reversibility in Algorithm 1

In (RM)HMC, one often chooses a hyperparameter $h > 0$ and sets the time horizon of the Hamiltonian dynamics as $h$, which motivates the design of Algorithm 1. However, under A1 and A2, we are not able to prove that the Hamiltonian dynamics (3) is defined at time $h > 0$, given any starting point $z_0 \in T^*M$ (see Proposition 3). This theoretical limitation requires to take some precautions in order to be properly define the Hamiltonian dynamics.

In the rest of this section, for any $z_0 \in T^*M$, we will denote by $z(\cdot, z_0) \in C^1(J_{z_0}, T^*M)$ the maximal solution to (3) with starting point $z_0$, uniquely defined in Proposition 2. For any $h > 0$, we recall below the definition of the sets $E_h$ and $\bar{E}_h$ the map $T_h$.

(a) The sets $E_h$ and $\bar{E}_h$ are defined by $E_h = \{ z \in T^*M : h < \sup J_z \}$ and $\bar{E}_h = \{ z \in E_h : h < \sup J_{(s \circ T_h)(z)} \}$, where $J$ is uniquely defined in Proposition 2. If $z_0 \in E_h$, then we are able to compute exactly the Hamiltonian dynamics (3) starting at $z_0$ up until time $h$. In addition, if $z_0 \in \bar{E}_h$, then we are also able to compute exactly the Hamiltonian dynamics (3) starting at $(s \circ T_h)(z_0)$ up until time $h$. Note that we have

$$\bar{E}_h = E_h \cap (s \circ T_h)^{-1}(E_h) .$$

(b) The map $T_h : E_h \to T^*M$ is such that $T_h(z_0) = z(h, z_0)$ for any $z_0 \in E_h$. If $z_0 \in \bar{E}_h$, then $T_h(z_0)$ outputs the state of the Hamiltonian dynamics at time $h$, starting from $z_0$.

We first prove that the restriction of $s \circ T_h$ to $\bar{E}_h$ is an involutive integrator, which is crucial to derive the “reversibility” of Algorithm 1 in Theorem 4.

Lemma 16. Assume A1, A2. Then, for any $h > 0$, $s \circ T_h$ is a $C^1$-diffeomorphism on $E_h$ such that $|\text{det.Jac}[s \circ T_h]| \equiv 1$.

Proof. Assume A1, A2. Let $h > 0$. It is clear that $T_h$ (and thus $s \circ T_h$) is well defined and continuously differentiable on $E_h$ (in particular on $E_h$), by elaborating on the proof of Proposition 2 combined with Cauchy-Lipschitz’s theorem. Let $z_0 \in \bar{E}_h$. By definition of $\bar{E}_h$, $T_h(z_0)$, resp. $J_{z_0}$, and $(T_h \circ s \circ T_h)(z_0)$, resp. $J_{(s \circ T_h)(z_0)}$, are well defined. We now aim to prove that $(T_h \circ s \circ T_h)(z_0) = s(z_0)$.

We define $z' : t \in [0, h] \to s(z(h - t, z_0))$, which existence is straightforward since $(h - t) \in J_{z_0}$ for any $t \in [0, h]$. In particular, $z'(0) = (s \circ T_h)(z_0)$ and $z'$ is a solution of the ODE (3) on the interval $[0, h]$. Yet, $[0, h] \subset J_{(s \circ T_h)(z_0)}$, and $z'(0) = z(0, (s \circ T_h)(z_0))$. Then, by unicity of $z(\cdot, (s \circ T_h)(z_0))$ (see Proposition 2), $z(\cdot, (s \circ T_h)(z_0))$ and $z'$ coincide on $[0, h]$. In particular, we have at time $h$

$$s(z_0) = z'(h) = z(h, (s \circ T_h)(z_0)) = (T_h \circ s \circ T_h)(z_0) .$$

Then for any $z_0 \in \bar{E}_h$, $(s \circ T_h \circ s \circ T_h)(z_0) = z_0$, i.e., $s \circ T_h$ is an involutive on $\bar{E}_h$. Since $s \circ T_h \in C^1(\bar{E}_h, T^*M)$, $s \circ T_h$ is a $C^1$-diffeomorphism on $\bar{E}_h$ such that $|\text{det.Jac}[s \circ T_h]| \equiv 1$.

We recall that we denote by $Q_c : T^*M \times B(T^*M) \to [0, 1]$, the transition kernel of the (homogeneous) Markov chain $(x_n, p_n)_{n \in [N]}$ generated by Algorithm 1. We also denote by:

(a) $Q_0 : T^*M \times B(T^*M) \to [0, 1]$, the transition kernel referring to Step 1 (also Step 3) in Algorithm 1.

(b) $Q_{c,1} : T^*M \times B(T^*M) \to [0, 1]$, the transition kernel referring to Step 2 in Algorithm 1.

We provide below details on Markov kernels $Q_0$, $Q_{c,1}$ and $Q_c$.

Kernel $Q_0$. This kernel corresponds to the Gaussian momentum update with refreshing rate $\beta$. For any $(z, z') \in T^*M \times T^*M$, we have

$$Q_0(z, dz') = N_x(p'; \sqrt{1 - \beta p, \beta Id}) dp' d\delta x(dx') = (2\pi\beta)^{-d/2} \text{det}(g(x))^{-1/2} \exp[-(2\beta)^{-1} \|p' - \sqrt{1 - \beta p}\|_{g(x)}^2] dp' d\delta x(dx') .$$

Kernel $Q_{c,1}$. This kernel is deterministic and corresponds to the exact integration of the Hamiltonian up until time $h$. For any $(z, z') \in T^*M \times T^*M$, we have

$$Q_{c,1}(z, dz') = 1_{\bar{E}_h}(z) \delta_{T_h(z)}(dz') + 1_{\bar{E}_h}(z) \delta_{x(z)}(dz') .$$
Kernel $Q_c$. This kernel corresponds to one step of Algorithm 1 (i.e., comprising Steps 1 to 3). For any $(z, z') \in T^*M \times T^*M$, we have

$$Q_c(z, dz') = \int_{T^*M \times T^*M} Q_0(z, dz_1) Q_{c,1}(z_1, dz_2) Q_0(z_2, dz').$$

We recall that $\bar{\pi}$, as defined in (2), admits a density with respect to the product Lebesgue measure given for any $z = (x, p) \in T^*M$ by

$$(d\bar{\pi}/(dx dp))(x, p) = (1/Z) \exp[-(1/2)\|p\|^2_{g(x)-1}] \det(g(x))^{-1/2} \exp[-V(x)].$$

Lemma 17. Assume A1. Then, the Markov kernel $Q_0$, defined in (21), is reversible (up to momentum reversal) with respect to $\bar{\pi}$.

Proof. Assume A1. For any $(z, z') \in T^*M \times T^*M$, we have

$$Q_0(z, dz')\bar{\pi}(dz) = (1/Z)(2\pi)^{-d/2} \bar{\beta}^{-d/2} \det(g(x))^{-1} \exp[-V(x)] dx dp \delta_z(dx')$$

$$\exp[-(2\bar{\beta})^{-1} \|p' - \sqrt{1 - \bar{\beta}} p\|^2_{g(x)-1}] \exp[-(1/2)\|p\|^2_{g(x)-1}]$$

$$= (1/Z)(2\pi)^{-d/2} \bar{\beta}^{-d/2} \det(g(x))^{-1} \exp[-V(x)] dx dp \delta_z(dx')$$

$$\exp[-(2\bar{\beta})^{-1} \{\|p\|^2_{g(x)-1} - 2\sqrt{1 - \bar{\beta}} (p', p)_{g(x)-1} + \|p\|^2_{g(x)-1}\}$$

$$= (1/Z)(2\pi)^{-d/2} \bar{\beta}^{-d/2} \det(g(x'))^{-1} \exp[-V(x')] dx dp \delta_z(dx')$$

$$\exp[-(2\bar{\beta})^{-1} \{\|p'\|^2_{g(x')-1} - 2\sqrt{1 - \bar{\beta}} (p, p')_{g(x')-1} + \|p\|^2_{g(x')-1}\}]$$

$$= Q_0(z', dz)\bar{\pi}(dz'),$$

which proves the reversibility of $Q_0$ with respect to $\bar{\pi}$. Since $s_{\#} Q_0 = Q_0$, we conclude the proof with Lemma 9.

Lemma 18. Assume A1, A2. Then, for any $h > 0$, the Markov kernel $Q_{c,1}$ with step-size $h$, defined in (22), is reversible up to momentum reversal with respect to $\bar{\pi}$.

Proof. Assume A1, A2. We recall that the set $\bar{E}_h$ is defined in (20). Let $f \in C(T^*M \times T^*M, \mathbb{R})$ with compact support. According to Definition 7, we aim to show that

$$\int_{T^*M \times T^*M} f(z, z') Q_{c,1}(z, dz')\bar{\pi}(dz) = \int_{T^*M \times T^*M} f(s(z'), s(z)) Q_{c,1}(z, dz')\bar{\pi}(dz).$$

We denote by $I$ the left integral of (24). We have $I = I_1 + I_2$ where

$$I_1 = \int_{\bar{E}_h} \bar{\pi}(z)f(z, T_h(z))dz,$$  
$$I_2 = \int_{\bar{E}_h} \bar{\pi}(z)f(z, s(z))dz.$$

We denote by $J$ the right integral of (24). By symmetry, we have $J = J_1 + J_2$ where

$$J_1 = \int_{\bar{E}_h} \bar{\pi}(z)f((s \circ T_h)(z), s(z))dz,$$  
$$J_2 = \int_{\bar{E}_h} \bar{\pi}(z)f(z, s(z))dz.$$

We directly have $I_2 = J_2$. Let us now prove that $I_1 = J_1$. By change of variable $z \mapsto (s \circ T_h)(z)$ in $I_1$, we have

$$I_1 = \int_{\bar{E}_h} \bar{\pi}(z)f(z, T_h(z))dz$$

$$= \int_{(s \circ T_h)(\bar{E}_h)} \bar{\pi}((s \circ T_h)(z))(s \circ T_h)(z), s(z))dz$$

(Lemma 16)

$$= \int_{\bar{E}_h} \bar{\pi}(z)f((s \circ T_h)(z), s(z))dz$$

(Proposition 2-(iv) & $(s \circ T_h)(\bar{E}_h) = \bar{E}_h$)

$$= J_1.$$

Finally, we obtain $I = J$ and thus prove (24) for any continuous function with compact support, which concludes the proof.

We are now ready to prove Theorem 4, which states that $Q_c$ is reversible up to momentum reversal with respect to $\bar{\pi}$.
Proof of Theorem 4. Assume A1, A2. Let $f : T^*M \times T^*M \to \mathbb{R}$ be a continuous function with compact support. We have

$$
\int_{T^*M \times T^*M} f(z, z') Q_c(z, dz') \bar{\pi}(dz)
= \int_{T^*M \times T^*M \times T^*M \times T^*M} f(z', z) Q_0(z, dz_1) Q_c(1)(z_1, dz_2) Q_0(z_2, dz') \bar{\pi}(dz)
$$

(see (23))

$$
= \int_{T^*M \times T^*M \times T^*M \times T^*M} f(s(z_1), s(z)) Q_0(z, dz_1) Q_c(1)(z, dz_2) Q_0(z_2, dz') \bar{\pi}(dz)
$$

(Lemma 17)

$$
= \int_{T^*M \times T^*M \times T^*M \times T^*M} f(s(z_1), z') Q_0(z_2, dz_1) Q_c(1)(z, dz_2) Q_0(z, dz') \bar{\pi}(dz)
$$

(momentum reversal on $z$)

(Lemma 18)

$$
= \int_{T^*M \times T^*M \times T^*M \times T^*M} f(s(z_1), s(z)) Q_0(z_2, dz_1) Q_c(1)(z', dz_2) Q_0(z, dz') \bar{\pi}(dz)
$$

(Lemma 17)

$$
= \int_{T^*M \times T^*M} f(s(z'), s(z)) Q_c(z, dz') \bar{\pi}(dz).
$$

Moreover, $s \# \bar{\pi} = \bar{\pi}$. Hence, by combining Definition 7 and Lemma 8, we obtain the result of Theorem 4. ∎

E Numerical integration in HMC

In this section, we first recall the definition of symplectic maps, and then discuss the choice of integrators in RMHMC. Finally, we focus on the implicit integrator defined in (4) and provide some notations, which will be notably used in appendix F.

Reminders on symplecticity. We define $J_d = \begin{pmatrix} 0 & I_d \\ -I_d & 0 \end{pmatrix} \in \mathbb{R}^{2d \times 2d}$.

Definition 19 (Hairer et al. (2006)). A linear mapping $A : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ is called symplectic if $A^\top J_d A = J_d$.

Definition 20 (Hairer et al. (2006)). A differentiable map $F : U \to \mathbb{R}^{2d}$, where $U \subset \mathbb{R}^{2d}$ is an open set, is called symplectic if the Jacobian matrix $\text{Jac}[F]$ is symplectic, i.e., if $\text{Jac}[F](z)^\top J_d \text{Jac}[F](z) = J_d$ for any $z \in U$. In particular, if $F$ is symplectic, then $|\det \text{Jac}[F]| \equiv 1$.

Choice of the integrators in RMHMC. Introducing a Riemannian metric $g$ in the Hamiltonian a priori makes it non separable. Thus, designing an integrator which is (i) symplectic, (ii) reversible and (iii) not too computationally heavy is challenging. The generalized Leapfrog integrator (GLI), or equivalently the Störmer-Verlet integrator, combined with fixed point iterations, as chosen by Girolami and Calderhead (2011), is considered as the standard scheme for RMHMC. Brofos and Lederman (2021b) analyze the impact of GLI on the ergodicity of RMHMC under a metric which is designed in the same manner as Cobb et al. (2019). In particular, they show that the convergence threshold used to compute the fixed-point process only matters to an extent, and identify a diminishing return to using smaller convergence thresholds. They compare the fixed-point approach with Newton’s method, which gives less iterations to converge. On the other hand, the implicit midpoint integrator (IMI) enjoys the same theoretical properties as GLI, when these two integrators are combined with fixed-point iterations. As shown by Brofos and Lederman (2021a), IMI may also show numerical advantages in terms of reversibility and volume preservation for specific target distributions. However, this integrator is hard to use for reversibility proofs due to its non-separability. Besides this, Cobb et al. (2019) combine a 2-state augmented Hamiltonian, based on the work of Tao (2016), with Strang splitting (Strang, 1968) to propose a symplectic explicit integrator which thus has the advantage not to rely on fixed-point iterations. Yet, this integrator does not satisfy reversibility in theory.

Details on the Störmer-Verlet integrator. The scheme defined in (4) can be written as $G_h = \tilde{G}_h \circ G_h$, where:

(a) $\tilde{G}_h : T^*M \to 2T^*M$ is the set-valued map implicitly defined by the first two equations of (4), i.e., for any $(z, z') \in T^*M \times T^*M$, $z' \in \tilde{G}_h(z)$ if and only if

$$
p' = p - \frac{b}{2} \partial_x H_2(x, p'), \quad x' = x + \frac{b}{2} \left[ \partial_p H_2(x, p') + \partial_x H_2(x', p') \right],
$$

(25)

We also define the map $g_{\tilde{G}_h} : T^*M \times T^*M \to \mathbb{R}^n \times \mathbb{R}^n$ by

$$
g_{\tilde{G}_h}(z, z') = (x' - x, -\frac{b}{2} \partial_x H_2(x, p') + \partial_p H_2(x', p'), p' - p + \frac{b}{2} \partial_x H_2(x, p')).
$$

(26)

such that $g_{\tilde{G}_h}(z, z') = 0$ if and only if $z' \in \tilde{G}_h(z)$.

(b) $G_h : T^*M \to T^*M$ is explicitly defined by the last equation of (4), i.e., for any $z \in T^*M$,

$$
G_h(z) = (x, p - \frac{b}{2} \partial_x H_2(x, p))
$$

(27)
F Proofs of Section 5.1

In this section, we state several results on the maps defined by the implicit integrators of the Hamiltonian (see Section 4.1), in order to prove Proposition 5.

Lemma 21. Let \( U \subset \mathbb{R}^d \) a non-empty open set and \( z \in U \). Assume there exist a neighbourhood \( U_z \subset U \) of \( z \), \( L > 0 \) and a \( L \)-Lipschitz-continuous map \( \psi : U \to \mathbb{R}^d \) such that \( \psi \in C^1(U_z, \mathbb{R}^d) \). Then, for any \( h \in (0, 1/L) \) and any \( a \in \mathbb{R}^d \), the map \( \psi_h : U \to \mathbb{R}^d \) defined for any \( z' \in U \) by \( \psi_h(z') = z' + h\psi(z') + a \) is a \( C^1 \)-diffeomorphism on a neighbourhood \( U'_z \subset U_z \) of \( z \).

Proof. Assume we are provided with \( U, z, U_z, L \) and \( \psi \) as described in Lemma 21. Let \( h \in (0, 1/L) \) and \( a \in \mathbb{R}^d \). We define the map \( \psi_h : U \to \mathbb{R}^d \) by \( \psi_h(z') = z' + h\psi(z') + a \), for any \( z' \in U_z \). Since \( \psi \in C^1(U_z, \mathbb{R}^d) \), it is clear that \( \psi_h \in C^1(U_z, \mathbb{R}^d) \). We have, for any \( z' \in U_z \), \( D\psi_h(z') = \text{Id} + hD\psi(z') \). In particular, for any \( w \in \mathbb{R}^d \), it comes that

\[
\|D\psi_h(w)\| \geq \|w\| - hL\|w\| = (1 - hL)\|w\|.
\]

Since \( 1 - hL > 0 \), \( \text{Jac}[\psi_h](z) \) is invertible. We conclude the proof by using the local inverse function theorem.

We recall that the set-valued map \( G_h \), defined in (4), is the generalized Leapfrog integrator, or equivalently the Störmer-Verlet integrator, of the non-separable Hamiltonian \( H_2 \) defined in Section 4.1. We state below a result of local smoothness of this integrator.

Lemma 22. Let \((M, g)\) be a a smooth manifold of \( \mathbb{R}^d \) and \( h > 0 \). Then, for any \((x(0), x(1)) \in M \times M\), the vector \( p^{(0)} \in T_{x(0)}^* M \) such that \((x(1), p^{(1)}) \in G_h(x(0), p^{(0)})\) for any \( p^{(1)} \in T_{x(1)}^* M \) is uniquely determined by \( p^{(0)} = G_{h,x(0)}(x(1))\), where the map \( G_{h,x(0)} : M \to T_{x(0)}^* M \) is defined by

\[
G_{h,x(0)}(y) = p^{(1/2)}(y) - \frac{h}{4}Dg(x(0))^\top[g(x(0))^{-1}p^{(1/2)}(y), g(x(0))^{-1}p^{(1/2)}(y)],
\]

with \( p^{(1/2)}(y) = \frac{1}{2}g(y)^{-1} + g(y)^{-1} - (y - x(0)) \). In particular, if \( g \in C^2(M, \mathbb{R}^{d \times d}) \), then, for any \( x(0) \in M \), \( G_{h,x(0)} \in C^1(M, T_{x(0)}^* M) \).

For any \( \alpha \geq 1 \), we define \( r^*_\alpha > 0 \) by

\[
r^*_\alpha = \min(1/50000, 1/(1000\alpha(\alpha + 1))).
\]

We recall that we denote by \( \mathcal{W}^0(x, r) \) the open Dikin ellipsoid (w.r.t. \( g \)) at \( x \in M \) of radius \( r > 0 \), given by \( \mathcal{W}^0(x, r) = \{ y \in \mathbb{R}^d : \|y - x\|_{g(x)} < r \} \). Assume A1, A2. Let \( x(0) \in M \) and \( r \in (0, r^*_\alpha) \), where \( \alpha \) is given by A2. Then, for any \( x \in \mathcal{W}^0(x(0), r) \), \( x \in M \) and \( \text{Jac}[G_{h,x(0)}](x) \) is invertible for any \( h > 0 \).

Proof. Let \((M, g)\) be a a smooth manifold of \( \mathbb{R}^d \) and \( h > 0 \). We first prove the existence and uniqueness of the map defined in (28). Let \((x(0), x(1)) \in M \times M \). We define for any \( y \in M \)

\[
p^{(1/2)}(y) = \frac{2}{h}(g(y)^{-1} + g(y)^{-1} - (y - x(0))), \quad \tilde{p}(y) = p^{(1/2)}(y) + \frac{h}{2}\partial_x H_2(x(0), p^{(1/2)}(y)).
\]

Note that these expressions are obtained by simply inverting the first two equations of (4). Then, by definition of \( G_h \), the vector \( p \in T_{x(1)}^* M \) such that \((x(1), p^{(1)}) \in G_h(x(0), p)\) for any \( p^{(1)} \in T_{x(1)}^* M \) is uniquely determined by \( p = \tilde{p}(x(1)) \). We thus obtain (28), using the expression of \( \partial_x H_2 \) given in Section 4.1. Moreover, it is clear that \( G_{h,x(0)} \) is continuously differentiable if \( g \in C^2(M, \mathbb{R}^{d \times d}) \).

We are now going to prove the second result of Lemma 22. Assume A1, A2. Let \( x(0) \in M \) and \( r \in (0, r^*_\alpha) \), where \( r^*_\alpha \) is defined in (29) and \( \alpha \) is given by A2. In particular \( r^*_\alpha \leq 1/11 \). For the sake of clarity, we will now denote \( g(x(0)) \) by \( g_0 \) for the rest of the proof.

We define the open Dikin ellipsoid \( B_0 = \mathcal{W}^0(x(0), r) \). Since \( r < 1 \), \( B_0 \subset M \) by Lemma 12-(b). Let \( h > 0 \). We now define the following maps on \( B_0 \)

\[
M_0 = \begin{cases} 
B_0 & \rightarrow S^d_+ (\mathbb{R}) \\
y & \rightarrow g_0^{-1} + g(y)^{-1}
\end{cases}, \quad K_0 = \begin{cases} 
B_0 & \rightarrow \mathbb{R}^d \\
y & \rightarrow g_0^{-1}M_0(y)^{-1}(y - x(0))
\end{cases}
\]
\[ \phi_0 = \left\{ \begin{array}{l l} B_0 & \rightarrow \mathbb{R}^d \\ y & \mapsto M_0(y)Dg_0[K_0(y), K_0(y)] \end{array} \right., \quad \tilde{\phi}_0 = \left\{ \begin{array}{l l} B_0 & \rightarrow \mathbb{R}^d \\ y & \mapsto \frac{1}{2}M_0(y)G_{n,x^0}(y) \end{array} \right.. \]

Note that we have, for any \( y \in B_0 \), \( \tilde{\phi}(y) = (y - x(0)) - \frac{1}{2}\tilde{\phi}_0(y) \). Since \( g \) is twice continuously differentiable on \( B_0 \), the maps previously defined are continuously differentiable. We now compute the derivatives of these maps. Let \( y \in B_0 \) and \( w \in \mathbb{R}^d \). We have:

\[
DM_0(y)[w] = -g(y)^{-1}Dg(y)[w]g(y)^{-1},
\]
\[
DK_0(y)[w] = -g_0^{-1}M_0(y)^{-1}DM_0(y)[w]M_0(y)^{-1}(y - x(0)) + \frac{\partial}{\partial y}M_0(y)^{-1}w
\]
\[
= -g_0^{-1}\{(g(y)g_0^{-1} + I_d)g(y)DM_0(y)[w]g(y)\}g_0^{-1}(y) + I_d\}^{-1}(y - x(0)) + \frac{\partial}{\partial y}M_0(y)^{-1}w
\]

\[
D\phi_0(y)[w] = DM_0(y)[w]Dg_0[K_0(y), K_0(y)] + M_0(y)Dg_0[DK_0(y)[w], K_0(y)] + M_0(y)Dg_0[K_0(y), DK_0(y)[w]],
\]
\[
D\tilde{\phi}_0(y)[w] = I_d - \frac{1}{2}D\phi_0(y)[w].
\]

We have in particular \( \tilde{\phi}_0(x(0)) = 0 \) and \( D\phi_0(x(0)) = 0 \). Let us first study the smoothness of \( D\phi_0 \) on \( B_0 \).

**Smoothness of** \( D\phi_0 \). We prove here that \( D\phi_0 \) is \( (r_0^*)^{-1} \)-Lipschitz-continuous on \( B_0 \) with respect to \( \| \cdot \|_{g_0} \). Let \( (y, y') \in B_0 \) and \( w \in \mathbb{R}^d \). We have

\[
\|D\phi_0(y)[w] - D\phi_0(y')[w]\|_{g_0} \leq \| DM_0(y)[w]Dg_0[K_0(y), K_0(y)] - DM_0(y')[w]Dg_0[K_0(y'), K_0(y')]\|_{g_0}
\]
\[
+ \| M_0(y)Dg_0[DK_0(y)[w], K_0(y)] - M_0(y')Dg_0[DK_0(y')[w], K_0(y')])\|_{g_0}
\]
\[
+ \| M_0(y)Dg_0[K_0(y), DK_0(y)[w]] - M_0(y')Dg_0[K_0(y'), DK_0(y')[w]]\|_{g_0}.
\]

Remark that the two last terms in (30) are very similar and can be bounded in the same way. The rest of the proof on the Lipschitz-continuity of \( D\phi_0 \) is separated in two steps, each of them consisting of bounding from above a term of (30).

**Step 1.** Let us first bound the first term in (30). For any \( x \in B_0 \), we denote \( DM_0(x)[w]Dg_0[K_0(x), K_0(x)] \) by \( a_1(x) \). We have

\[
g_0^{1/2}(a_1(y) - a_1(y')) = \{ g_0^{1/2}(DM_0(y)[w] - DM_0(y')[w])g_0^{1/2}\} \{ g_0^{1/2}Dg_0[K_0(y), K_0(y)]\}
\]
\[
\quad + \{ g_0^{1/2}Dg_0(y)[w]g_0^{1/2}\} \{ g_0^{1/2}Dg_0[K_0(y), K_0(y)] - Dg_0[K_0(y'), K_0(y')])\}. \tag{31}
\]

We now aim to bound each one of the four terms that appear in (31).

**Step 1.1.** First, we have

\[
g_0^{1/2}(DM_0(y)[w] - DM_0(y')[w])g_0^{1/2} = g_0^{1/2}(g(y')^{-1}Dg(y')[w]g(y')^{-1} - g(y)^{-1}Dg(y)[w]g(y)^{-1})g_0^{1/2}
\]
\[
= g_0^{1/2}(g(y')^{-1} - g(y)^{-1})Dg(y)[w]g(y')^{-1}g_0^{1/2}
\]
\[
+ g_0^{1/2}(Dg(y')[w] - Dg(y)[w])g(y')^{-1}g_0^{1/2}
\]
\[
+ g_0^{1/2}g(y)^{-1}Dg(y)[w]g(y)^{-1} - g(y)^{-1})g_0^{1/2}.
\]

We recall that \( r \leq r_0^* \leq 1/11 \), and thus, we have for any \( x \in \{ y, y' \} \) the following inequalities

\[
\|g_0^{1/2}\{g(y')^{-1} - g(y)^{-1}\}g_0^{1/2}\|_2 \leq 3(1 - r)^{-3}\|y - y\|_{g_0}, \quad \text{(on the model of (14))}
\]
\[
\|g_0^{1/2}g(x)^{-1}g_0^{1/2}\|_2 \leq (1 - r)^{-2}, \quad \text{(Lemma 12-(b))}
\]
\[
\|g_0^{1/2}Dg(x)[w]g_0^{1/2}\|_2 \leq (1 - r)^{-2}\|g(x)^{-1/2}Dg(x)[w]g(x)^{-1/2}\|_2.
\]

In particular, we have for any \( x \in \{ y, y' \} \)

\[
\|g(x)^{-1/2}Dg(x)[w]g(x)^{-1/2}\|_2 = \sup_{\{w' \in \mathbb{R}^d : \|w'\|_2 = 1\}} \|Dg(x)[w, g(x)^{-1/2}w']\|_{g(x)^{-1}}. \tag{32}
\]
Thus, by using (32) and (33), we have

\[ \|g(y)^{-1/2}(Dg(y')|w) - Dg(y)|w)\|g(y)^{-1/2}\|_2 \]

and using again that \( r \leq r^*_a \leq 1/11 \), we have

\[ \|g(y)^{-1/2}(Dg(y')|w) - Dg(y)|w)\|g(y)^{-1/2}\|_2 \]

Thus, by using (32) and (33), we have

\[ \|\mathbf{g}_0^{1/2}(DM_0(y)|w) - DM_0(y')|w)\|\|_2 \leq (12(1 - r)^{-8} + 5\alpha(\alpha + 1)/3(1 - r)^{-6})\|y - y'\|\|_2\|_2. \]

**Step 1.2.** Secondly, we have

\[ \|\mathbf{g}_0^{-1/2}D_0|K_0(y), K_0(y)\|_2 \leq 2\|K_0(y)\|\|_2 \]

where we have by Lemma 12-(b)

\[ \mathbf{g}_0^{-1/2}M_0(y)^{-1}\|\mathbf{g}_0\leq 1 + (1 - r)^{-2}I_d. \]

Thus, we obtain

\[ \|\|\mathbf{g}_0^{-1/2}D_0|K_0(y), K_0(y)\|\|_2 \leq 2(1 - r)^{-3}\|w\|\|_2. \]

**Step 1.3.** Thirdly, we have

\[ \|\mathbf{g}_0^{1/2}DM_0(y')|w)\|\|_2 \leq (1 - r)^{-2}\|\mathbf{g}(x)^{-1/2}Dg(y')|w)\|\|_2 \]

\[ \leq 2(1 - r)^{-3}\|w\|\|_2. \]

**Step 1.4.** Fourthly, we have

\[ \|\mathbf{g}_0^{-1/2}(Dg_0|K_0(y), K_0(y') - Dg_0|K_0(y'), K_0(y)|)\|_2 \]

In particular, \( M_0(y)^{-1}(y - x^{(0)}) - M_0(y')^{-1}(y' - x^{(0)}) = M_0(y)^{-1}(y - y') + (M_0(y)^{-1} - M_0(y')^{-1})(y' - x^{(0)}) \), and thus we have

\[ \|M_0(y)^{-1}(y - x^{(0)}) - M_0(y')^{-1}(y' - x^{(0)})\|\|_2 \]

\[ \leq \|\mathbf{g}_0^{-1/2}M_0(y)^{-1}\|\|_2\|y - y'\|\|_2 + r\|\mathbf{g}_0^{1/2}(M_0(y)^{-1} - M_0(y')^{-1})\|\|_2 \]

\[ \leq (1 + (1 - r)^2)^{-1}\|y - y'\|\| + r\|\mathbf{g}_0^{1/2}(M_0(y)^{-1} - M_0(y')^{-1})\|\|_2. \]

(assuming 34)
We now aim to find an upper bound for \( \|g_0^{-1/2}(M_0(y)^{-1} - M_0(y')^{-1})g_0^{-1/2}\|_2 \). We have
\[
\begin{align*}
g_0^{-1/2}(M_0(y)^{-1} - M_0(y')^{-1})g_0^{-1/2}
 &= (I_d + g_0^{-1/2}g(y)^{-1}g_0^{-1/2})^{-1} - (I_d + g_0^{-1/2}g(y')^{-1}g_0^{-1/2})^{-1} \\
 &= (I_d + g_0^{-1/2}g(y')^{-1}g_0^{-1/2} + g_0^{-1/2}(g(y)^{-1} - g(y')^{-1})g_0^{-1/2})^{-1} - (I_d + g_0^{-1/2}g(y')^{-1}g_0^{-1/2})^{-1} \\
 &= B(y')^{-1/2}(I_d + B(y')^{-1/2}g_0^{-1/2}(g(y)^{-1} - g(y')^{-1})g_0^{-1/2}B(y')^{-1/2} - I_d)B(y')^{-1/2},
\end{align*}
\]
where \( B(y') = I_d + g_0^{-1/2}g(y')^{-1}g_0^{-1/2} \). In particular, \( (1 + (1 - r)^{-2})^{-1/2}I_d \leq B(y')^{-1/2} \leq (1 + (1 - r)^{-2})^{-1/2}I_d \) by Lemma 12-(b). Note that (13) still holds, where \( x, x' \) and \( r \) are respectively replaced by \( y, y' \) and \( r \). Thus, on the model on (14), we have
\[
\{(1 - \|y' - y\|_{g(y)})^2 - 1\}(1 - r)^2I_d \leq g_0^{-1/2}\{g(y)^{-1} - g(y')^{-1}\}g_0^{-1/2} \leq \{(1 - \|y' - y\|_{g(y)})^2 - 1\}(1 - r)^{-2}I_d,
\]
and then
\[
\begin{align*}
(1 + \{(1 - \|y' - y\|_{g(y)})^2 - 1\}(1 - r)^2(1 + (1 - r)^{-2})^{-1})I_d \\
\leq I_d + B(y')^{-1/2}g_0^{-1/2}\{g(y)^{-1} - g(y')^{-1}\}g_0^{-1/2}B(y')^{-1/2} \\
\leq (1 + \{(1 - \|y' - y\|_{g(y)})^2 - 1\}(1 - r)^{-2}(1 + (1 - r)^{-2})^{-1})I_d.
\end{align*}
\]
Therefore, we have \( \|g_0^{-1/2}(M_0(y)^{-1} - M_0(y')^{-1})g_0^{-1/2}\|_2 \leq (1 + (1 - r)^{-2})^{-1} \max(\|f_1(r)\|, \|f_2(r)\|) \) where
\[
\begin{align*}
f_1(r) &= (1 + \{(1 - \|y' - y\|_{g(y)})^2 - 1\}(1 - r)^{-2}(1 + (1 - r)^{-2})^{-1})^{-1} - 1, \\
f_2(r) &= (1 + \{(1 - \|y' - y\|_{g(y)})^2 - 1\}(1 - r)^{-2}(1 + (1 - r)^{-2})^{-1})^{-1} - 1.
\end{align*}
\]
We now aim to control the upper bound \( \max(\|f_1(r)\|, \|f_2(r)\|). \)

(a) We first bound \( |f_1(r)|. \) Since \( \|y' - y\|_{g(y)} \geq 0 \), it is clear that \( f_1(r) \leq 0 \). Using Inequality (a) with \( u = \|y' - y\|_{g(y)} \), where \( u \leq 1/5 \) by (13), we obtain
\[
|f_1(r)| = -f_1(r) \\
\leq 1 - (1 + 3(1 - r)^{-2}(1 + (1 - r)^{-2})^{-1}\|y' - y\|_{g(y)})^{-1} \\
\leq 3(1 - r)^{-2}(1 + (1 - r)^{-2})^{-1}\|y' - y\|_{g(y)} \quad \text{(Inequality (d))} \\
\leq 3(1 - r)^{-3}(1 + (1 - r)^{-2})^{-1}\|y' - y\|_{g_0}. \quad \text{(Lemma 12-(c))}
\]

(b) We now bound \( f_2(r) \). We have
\[
\begin{align*}
f_2(r) &\leq (1 - 2(1 - r)^2(1 + (1 - r)^{-2})^{-1}\|y' - y\|_{g(y)})^{-1} - 1 \\
&\leq 4(1 - r)^2(1 + (1 - r)^{-2})^{-1}\|y' - y\|_{g(y)} \\
&\leq 4(1 - r)(1 + (1 - r)^{-2})^{-1}\|y' - y\|_{g_0} \quad \text{(Lemma 12-(c))}
\end{align*}
\]
where we used (i) Inequality (d) in the first line with \( u = \|y' - y\|_{g(y)} \), and (ii) Inequality (b) in the second line with \( u = 2(1 - r)^2(1 + (1 - r)^{-2})^{-1}\|y' - y\|_{g(y)} \leq 4r(1 - r)(1 + (1 - r)^{-2})^{-1} \leq 1/2 \) with \( r \leq 1/11 \).

We recall that \( r \in (0, 1) \), and thus, we have respectively \( (1 - r)^{-3} \geq (1 - r) \) and \( (1 + (1 - r)^{-2})^{-1} \geq (1 + (1 - r)^{-2})^{-1} \). Therefore, \( \max(|f_1(r)|, |f_2(r)|) \leq (4/3)|f_1(r)| \) and
\[
\begin{align*}
\|g_0^{-1/2}(M_0(y')^{-1} - M_0(y)^{-1})g_0^{-1/2}\|_2 &\leq 4(1 - r)^3(1 + (1 - r)^{-2})^{-1}\|y' - y\|_{g_0}, \\
\|K_0(y) - K_0(y')\|_{g_0} &\leq (1 + (1 - r)^{-2})^{-1}\{1 + 4r(1 - r)^{-3}(1 + (1 - r)^{-2})^{-1}\}\|y' - y\|_{g_0}.
\end{align*}
\]
By combining (37), (38) and (39), we finally have
\[
\|g_0^{-1/2}(Dg_0[K_0(y), K_0(y)] - Dg_0[K_0(y'), K_0(y')])\|_2
\]
Conclusion of Step 1. By combining the results of Steps 1.1 to 1.4, it comes that
\[
\|DM_0(y)[w]Dg_0[K_0(y), K_0(y)] - DM_0(y')[w]Dg_0[K_0(y'), K_0(y')]\|_{g_0} \\
= \|g_0^{1/2}(a_1(y) - a_1(y'))\|_2 \\
\leq \{2r^2(1 + (1 - r)^2)^{-2}(1 + (1 - r)^2)^{-3}(1 + (1 - r)^2)^{-1}\}^2\|y - y'\|_{g_0}.
\]

Step 2. Let us now bound the second term in (30). For any \(x \in B_0\), we denote \(M_0(y)Dg_0[DK_0(y)[w], K_0(y)]\) by \(a_2(x)\). We have
\[
g_0^{1/2}(a_2(y) - a_2(y')) = \{g_0^{1/2}(M_0(y) - M_0(y'))g_0^{1/2}\} \{g_0^{-1/2}Dg_0[DK_0(y)[w], K_0(y)]\} \\
+ \{g_0^{1/2}M_0(y')g_0^{1/2}\} \{g_0^{1/2}(Dg_0[DK_0(y)[w], K_0(y)] - Dg_0[DK_0(y')[w], K_0(y')]\}.
\]

We now aim to bound each of the four terms that appear in (40).

Step 2.1. First, we have
\[
\|g_0^{1/2}(M_0(y) - M_0(y'))g_0^{1/2}\|_2 = \|g_0^{1/2}(g(y)^{-1} - g(y')^{-1})g_0^{1/2}\|_2 \\
\leq 3(1 - r)^{-3}\|y - y'\|_{g_0}.
\]
(on the model of (14))

Step 2.2. Secondly, we have
\[
\|g_0^{-1/2}Dg_0[DK_0(y)[w], K_0(y)]\|_2 \leq 2\|DK_0(y)[w]\|_{g_0}\|M_0(y)^{-1}(y - x^{(0)})\|_{g_0^{-1}}. 
\]
\[(\text{Lemma 12-(a)})\]
\[
\leq 2r(1 + (1 - r)^2)^{-1}\|DK_0(y)[w]\|_{g_0}, 
\]
(see Step 2.2.)

where
\[
\|DK_0(y)[w]\|_{g_0} \leq \|g_0^{-1/2}(g(y)g_0^{-1} + I_d)^{-1}g_0^{1/2}\|_2\|g_0^{-1/2}g(y)^{1/2}\|_2\|g(y)^{-1/2}Dg_0[y]\|g(y)^{-1/2}||w||_{g_0} + \|M_0(y)^{-1}w\|_{g_0^{-1}}.
\]

Using (32) and (34), it comes that
\[
\|DK_0(y)[w]\|_{g_0} \leq \{2r(1 - r)^{-3}(1 + (1 - r)^2)^{-2} + (1 + (1 - r)^2)^{-1}\}\|w\|_{g_0}.
\]

Then, we have
\[
\|g_0^{-1/2}Dg_0[DK_0(y)[w], K_0(y)]\|_2 \leq 2r(1 + (1 - r)^2)^{-2}\{1 + 2r(1 - r)^{-3}(1 + (1 - r)^2)^{-1}\}\|w\|_{g_0}.
\]

Step 2.3. Thirdly, we have \(\|g_0^{1/2}M_0(y')g_0^{1/2}\|_2 = \|g_0^{1/2}g(y')^{-1}g_0^{1/2} + I_d\|_2 \leq 1 + (1 - r)^{-2}.
\]

Step 2.4. Fourthly, using Lemma 12-(a), we have
\[
\|g_0^{-1/2}(Dg_0[DK_0(y)[w], K_0(y)] - Dg_0[DK_0(y')[w], K_0(y')]\|_2 \\
\leq 2\|DK_0(y)[w] - DK_0(y')[w]\|_{g_0}\|K_0(y)\|_{g_0} + 2\|DK_0(y)[w]\|_{g_0}\|K_0(y) - K_0(y')\|_{g_0}.
\]
We recall that the following inequalities hold

\[ \|K_0(y)\|_{\|\cdot\|_0} \leq (1 + (1 - r)^2)^{-1}, \]
\[ \|DK_0(y)[w]\|_{\|\cdot\|_0} \leq (1 + (1 - r)^2)^{-1} \{ 1 + 2r(1 - r)^{-3}(1 + (1 - r)^2)^{-1} \} \|w\|_{\|\cdot\|_0}, \]
\[ \|K_0(y) - K_0(y')\|_{\|\cdot\|_0} \leq (1 + (1 - r)^2)^{-1} \{ 1 + 4r(1 - r)^{-3}(1 + (1 - r)^2)^{-1} \} \|y' - y\|_{\|\cdot\|_0}. \]

We are now going to bound \( \|DK_0(y)[w] - DK_0(y')[w]\|_{\|\cdot\|_0}. \) We have

\[ \|DK_0(y)[w] - DK_0(y')[w]\|_{\|\cdot\|_0} \leq (M_0(y)^{-1} - M_0(y')^{-1})w\|_{\|\cdot\|_0} + A_1 + A_2 + A_3 + A_4, \]

where

\[ A_1 = \| (I_d + \varrho_0^{-1/2}g(y)\varrho_0^{-1/2})^{-1} - (I_d + \varrho_0^{-1/2}g(y')\varrho_0^{-1/2})^{-1} \|_2, \]
\[ \times \varrho_0^{-1/2}Dg(y)[w]\|_{\|\cdot\|_0}^{-1/2} (I_d + \varrho_0^{-1/2}g(y)\varrho_0^{-1/2})^{-1} \varrho_0^{-1/2}y(0)^{1/2} \|_2, \]
\[ A_2 = \| (I_d + \varrho_0^{-1/2}g(y')\varrho_0^{-1/2})^{-1} - (I_d + \varrho_0^{-1/2}g(y)\varrho_0^{-1/2})^{-1} \|_2, \]
\[ \times \{ (I_d + \varrho_0^{-1/2}g(y')\varrho_0^{-1/2})^{-1} - (I_d + \varrho_0^{-1/2}g(y)\varrho_0^{-1/2})^{-1} \} \varrho_0^{1/2}y(0)^{1/2} \|_2, \]
\[ A_3 = \| (I_d + \varrho_0^{-1/2}g(y')\varrho_0^{-1/2})^{-1} - (I_d + \varrho_0^{-1/2}g(y)\varrho_0^{-1/2})^{-1} \|_2, \]
\[ \times \{ (I_d + \varrho_0^{-1/2}g(y')\varrho_0^{-1/2})^{-1} - (I_d + \varrho_0^{-1/2}g(y)\varrho_0^{-1/2})^{-1} \} \varrho_0^{-1/2}y(0)^{-1/2} \|_2. \]

In particular, we have

\[ \| (M_0(y)^{-1} - M_0(y')^{-1})w\|_{\|\cdot\|_0} \leq 4(1 - r)^{-3}(1 + (1 - r)^2)^{-2} \|y' - y\|_{\|\cdot\|_0} \|w\|_{\|\cdot\|_0}, \] (using (39))
\[ \max(A_1, A_3) \leq 8r(1 - r)^{-6}(1 + (1 - r)^2)^{-3} \|y' - y\|_{\|\cdot\|_0} \|w\|_{\|\cdot\|_0}, \] (using (32), (34) and (39))
\[ A_2 \leq 5\alpha(\alpha + 1)/3r(1 - r)^{-4}(1 + (1 - r)^2)^{-2} \|y' - y\|_{\|\cdot\|_0} \|w\|_{\|\cdot\|_0}, \] (using (33) and (34))
\[ A_4 \leq 2(1 - r)^{-3}(1 + (1 - r)^2)^{-2} \|y' - y\|_{\|\cdot\|_0} \|w\|_{\|\cdot\|_0}. \] (using (32) and (34))

Therefore, we have

\[ \|g_0^{1/2}(DK_0(y)[w], K_0(y) - Dg_0[DK_0(y')[w], K_0(y')]\|_2 \]
\[ \leq 2r(1 + (1 - r)^2)^{-1} \{ 3 + 4r(1 - r)^{-3}(1 + (1 - r)^2)^{-1} \} \]
\[ \times \{ 4(1 - r)^{-3}(1 + (1 - r)^2)^{-2} + 16r(1 - r)^{-6}(1 + (1 - r)^2)^{-3} \}
\[ + 5\alpha(\alpha + 1)/3r(1 - r)^{-4}(1 + (1 - r)^2)^{-2} + 2(1 - r)^{-3}(1 + (1 - r)^2)^{-2} \} \|y' - y\|_{\|\cdot\|_0} \|w\|_{\|\cdot\|_0}
\[ + 2\{ 1 + 2r(1 - r)^{-3}(1 + (1 - r)^2)^{-1} \}
\[ \times (1 + (1 - r)^2)^{-2}(1 + 4r(1 - r)^{-3}(1 + (1 - r)^2)^{-1}) \|y' - y\|_{\|\cdot\|_0} \|w\|_{\|\cdot\|_0}. \]

Conclusion of Step 2. By combining the results of Steps 2.1 to 2.4, it comes that

\[ \|M_0(y)Dg_0[DK_0(y)[w], K_0(y) - M_0(y')Dg_0[DK_0(y')[w], K_0(y')]\|_{\|\cdot\|_0}
\[ = \|g_0^{1/2}(a_2(y) - a_2(y'))\|_2 \]
\[ \leq \{ 6r(1 - r)^{-3}(1 + (1 - r)^2)^{-2}[1 + 2r(1 - r)^{-3}(1 + (1 - r)^2)^{-1}]
\[ + 2r(1 + (1 - r)^{-2})(1 + (1 - r)^2)^{-1}[3 + 4r(1 - r)^{-3}(1 + (1 - r)^2)^{-1}]
\[ \times \{ 4(1 - r)^{-3}(1 + (1 - r)^2)^{-2} + 16r(1 - r)^{-6}(1 + (1 - r)^2)^{-3} \}
\[ + 5\alpha(\alpha + 1)/3r(1 - r)^{-4}(1 + (1 - r)^2)^{-2} + 2(1 - r)^{-3}(1 + (1 - r)^2)^{-2} \}
\[ \times (1 + (1 - r)^2)^{-2}(1 + 4r(1 - r)^{-3}(1 + (1 - r)^2)^{-1}) \|y' - y\|_{\|\cdot\|_0} \|w\|_{\|\cdot\|_0}. \]
Conclusion. Finally, we have 
\[
\|D\phi_0(y)[w] - D\phi_0(y')[w]\|_{g_0} \leq c(r)\|y - y'\|_{g_0}\|w\|_{g_0},
\]
where 
\[
c(r) \leq 24r^2(1 - r)^{-12} + 10\alpha(\alpha + 1)/3r^2(1 - r)^{-10}
+ 32r(1 - r)^{-7} + 128r^2(1 - r)^{-12} + 128r^3(1 - r)^{-17}
+ 48r(1 - r)^{-9} + 192r^2(1 - r)^{-14} + 20\alpha(\alpha + 1)r^2(1 - r)^{-10} + 24r(1 - r)^{-9}\{1 + (1 - r)^{-2}\}
+ \{64r^2(1 - r)^{-14} + 256r^3(1 - r)^{-19} + 80\alpha(\alpha + 1)/3r^3(1 - r)^{-15} + 32r^2(1 - r)^{-14}\}\{1 + (1 - r)^{-2}\},
\]
by combining the results of Step 1 (two first lines) and Step 2 (following lines). Hence, using that \(r \leq 1/11\), we have 
\[
c(r) \leq \max(24 \times 256, 5 \times 80\alpha(\alpha + 1)/3)(1 - r)^{-21}
\leq \max(6144, 400\alpha(\alpha + 1)/3)15/2
\leq \max(46080, 1000\alpha(\alpha + 1))
\leq 1/r^*_\alpha, \quad \text{(see }29\text{)}
\]
i.e., for any \((y, y') \in B_0 \times B_0\) and \(w \in \mathbb{R}^d\), we have 
\[
\|D\phi_0(y)[w] - D\phi_0(y')[w]\|_{g_0} \leq (r^*_\alpha)^{-1}\|y - y'\|_{g_0}\|w\|_{g_0},
\]
and thus 
\[
\|D\phi_0(y) - D\phi_0(y')\|_{g_0} \leq (r^*_\alpha)^{-1}\|y - y'\|_{g_0}.
\]
This last inequality finally proves that \(D\phi_0\) is \((r^*_\alpha)^{-1}\)-Lipschitz-continuous on \(B_0\) with respect to \(\|\cdot\|_{g_0}\).

**Inequality on \(D\tilde{\phi}_0\).** Elaborating on the smoothness of \(D\phi_0\), we prove here that \(\|D\tilde{\phi}_0(y)\|_{g_0} > 1/2\) for any \(y \in B_0\). Let \(y \in B_0\), we have 
\[
\|I_1\|_{g_0} = \|D\tilde{\phi}_0(y) + 1/2D\phi_0(y)\|_{g_0},
1 \leq \|D\tilde{\phi}_0(y)\|_{g_0} + 1/2\|D\phi_0(y)\|_{g_0},
1 - 1/2\|D\phi_0(y)\|_{g_0} \leq \|D\tilde{\phi}_0(y)\|_{g_0}.
\]
We recall that \(D\phi_0(x^{(0)}) = 0\) and that \(D\phi_0\) is \((r^*_\alpha)^{-1}\)-Lipschitz-continuous on \(B_0\), Thus, we obtain 
\[
\|D\phi_0(y)\|_{g_0} = \|D\phi_0(y) - D\phi_0(x^{(0)})\|_{g_0} \leq (r^*_\alpha)^{-1}\|y - x^{(0)}\|_{g_0} < (r^*_\alpha)^{-1}r \leq 1,
\]
and then \(\|D\tilde{\phi}_0(y)\|_{g_0} > 1/2\), which proves the result.

**Smoothness of \(\phi_0\) and \(\tilde{\phi}_0\).** We prove here that \(\phi_0\) (and thus \(\tilde{\phi}_0\)) is Lipschitz-continuous on \(B_0\) with respect to \(\|\cdot\|_{g_0}\). Let \((y, y') \in B_0 \times B_0\). We have 
\[
\|\phi_0(y) - \phi_0(y')\|_{g_0} \leq \|\{M_0(y) - M_0(y')\}Dg_0[K_0(y), K_0(y)]\|_{g_0}
+ \|M_0(y')\{Dg_0[K_0(y), K_0(y)] - Dg_0[K_0(y'), K_0(y')]\}\|_{g_0}.
\]
To prove the Lipschitz-continuity of \(\phi_0\), we are going to proceed in two steps, each of them consisting of bounding from above a term of \((41)\).

**Step 1.** Let us first bound the first term in \((41)\). Since \(r \leq 1/11\), we have 
\[
\|\{M_0(y) - M_0(y')\}Dg_0[K_0(y), K_0(y)]\|_{g_0}
\]
Step 2. Let us now bound the second term in (41). We have

\[ \| M_0(y') \{ D g_0 [K_0(y), K_0(y)] - D g_0 [K_0(y'), K_0(y')] \} \|_{g_0} \]

\[ \leq \| g_0^{1/2} M_0(y') g_0^{1/2} \|_2 \| D g_0 [K_0(y), K_0(y)] \|_{g_0}^{-1} \]

\[ \leq 3(1 - r)^{-3} \| y - y' \|_{g_0} \times 2 \| K_0(y) \|_{g_0}^2 \]

\[ \leq 6r^2(1 - r)^{-3}(1 + (1 - r)^2)^{-2} \| y - y' \|_{g_0} . \]

(see (14) and Lemma 12-(a))

where we recall that the following inequalities hold

\[ \| K_0(y) \|_{g_0} \leq r(1 + (1 - r)^2)^{-1} , \]

\[ \| K_0(y) - K_0(y') \|_{g_0} \leq (1 + (1 - r)^2)^{-1} \{ 1 + 4r(1 - r)^{-3}(1 + (1 - r)^2)^{-1} \} \| y' - y \|_{g_0} . \]

Thus, we have

\[ \| M_0(y') \{ D g_0 [K_0(y), K_0(y)] - D g_0 [K_0(y'), K_0(y')] \} \|_{g_0} \]

\[ \leq 4r \{ 1 + (1 - r)^2 \}^{-2} \{ 1 + 4r(1 - r)^{-3}(1 + (1 - r)^2)^{-1} \} \| y - y' \|_{g_0} . \]

Conclusion. Since \( r \leq 1/11 \), we finally have

\[ \| \phi_0(y) - \phi_0(y') \|_{g_0} \leq \{ 6r^2(1 - r)^{-3}(1 + (1 - r)^2)^{-2} \]

\[ + 4r \{ 1 + (1 - r)^2 \}^{-2} \{ 1 + 4r(1 - r)^{-3}(1 + (1 - r)^2)^{-1} \} \| y - y' \|_{g_0} \]

\[ \leq \{ 6r^2(1 - r)^{-7} + 4r(1 - r)^{-4} + 32r^2(1 - r)^{-9} + 64r^2(1 - r)^{-14} \} \| y - y' \|_{g_0} \]

\[ \leq 4 \times 64r(1 - r)^{-14} \| y - y' \|_{g_0} \]

\[ \leq 4864/5r \| y - y' \|_{g_0} . \]

Therefore, \( \phi_0 \) and \( \hat{\phi}_0 \) are respectively \( (4864/5r) \) and \( (1 + 2432/5r) \)-Lipschitz-continuous on \( B_0 \) with respect to \( \| \cdot \|_{g_0} \).

We are now ready to prove the second result of Lemma 22.

Invertibility of \( \text{Jac}[G_{h,x(o)}] \). Let \( x \in B_0 \) and \( w \in \mathbb{R}^d \). We have \((h/2)G_{h,x(o)} = M_0(y)^{-1} \phi_0(y) \) and thus,

\[ (h/2)DG_{h,x(o)}(x)[w] = M_0(x)^{-1} D\hat{\phi}_0(x)[w] + DM_0(x)^{-1}[w]\hat{\phi}_0(x) , \]

\[ D\hat{\phi}_0(x)[w] = (h/2)M_0(x)DG_{h,x(o)}(x)[w] - M_0(x)DM_0(x)^{-1}[w]\hat{\phi}_0(x) . \]

Then, we have

\[ \| D\hat{\phi}_0(x)[w] \|_{g_0} \leq (h/2)\| g_0^{1/2} M_0(x) g_0^{1/2} \|_2 \| D G_{h,x(o)}(x)[w] \|_{g_0}^{-1} \]

\[ + \| g_0^{1/2} M_0(x) g_0^{1/2} \|_2 \| g_0^{-1/2} D M_0(x)^{-1}[w] \|_{g_0}^{-1} \| \hat{\phi}_0(x) \|_{g_0} \]

\[ \leq \{ 1 + (1 - r)^{-2} \} \{ (h/2)\| D G_{h,x(o)}(x)[w] \|_{g_0}^{-1} + \| g_0^{-1/2} D M_0(x)^{-1}[w] \|_{g_0}^{-1/2} \| \hat{\phi}_0(x) \|_{g_0} \} , \]

where \( DM_0(x)^{-1}[w] = -M_0(x)^{-1} DM_0(x)[w] M_0(x)^{-1} \) and

\[ \| g_0^{-1/2} DM_0(x)^{-1}[w] g_0^{-1/2} \|_2 \leq \| g_0^{-1/2} M_0(x)^{-1} g_0^{-1/2} \|_2 \| g_0^{-1/2} D M_0(x)[w] g_0^{-1/2} \|_2 \]

\[ \leq 2(1 - r)^{-3}(1 + (1 - r)^2)^{-1} \| w \|_{g_0} . \]

(see (36))
\[ \leq 2(1-r)^{-7}\|w\|_{g_0}. \]

Moreover, using the Lipschitz-continuity of \(\tilde{\phi}_0\) on \(B_0\) and \(\tilde{\phi}_0(x^{(0)}) = 0\), we have
\[
\|\tilde{\phi}_0(x)\|_{g_0} \leq \|\tilde{\phi}_0(x) - \tilde{\phi}_0(x^{(0)})\|_{g_0} + \|\tilde{\phi}_0(x^{(0)})\|_{g_0} \leq (1 + 2432/5r)\|x - x^{(0)}\|_{g_0} < (1 + 2432/5r)r. \tag{44}
\]

Since \(r \leq 1/11\), we have \(1 + (1-r)^{-2} \leq 5/2\), and by combining (42),(43) and (44), we obtain
\[
\|D\tilde{\phi}_0(x)[w]\| \leq (5h/4)\|DG_{h,x^{(0)}}(x)[w]\|_{\tilde{g}_0^{-1}} + 4874(1-r)^{-7}r\|w\|_{g_0}.
\]

Since \(\|D\tilde{\phi}_0(x)[w]\|_{g_0} > \|w\|_{g_0}/2\) and \((1-r)^{-7} \leq 2\) with \(r \leq 1/11\), the last inequality becomes
\[
(5h/4)\|DG_{h,x^{(0)}}(x)[w]\|_{\tilde{g}_0^{-1}} \geq \{1/2 - 9748r\}\|w\|_{g_0},
\]
\[
\geq 1/2 - r/(4r^*_0) \geq 1/4. \tag{see (29)}
\]

In particular, \(\text{Jac}[G_{h,x^{(0)}}(x)]\) is invertible, which concludes the proof. \qed

We prove below that, for any \(z^{(0)} \in T^*M\), the set \(G_h(z^{(0)})\) is reduced to a single point, for \(h\) small enough depending on \(z^{(0)}\).

**Lemma 23.** For any \(w \geq 0\), any \(r \in (0,1)\) and any \(\alpha \geq 1\), we define
\[
h_1(w,r,\alpha) = \min \left( \frac{1}{1 + (1-r)^{-2} + 2(2r + w)}, \frac{(1-r)^3}{(r+w)(1+3r/2) + 1/2(r+w)^2} \right). \tag{45}
\]

We recall that the set-valued map \(G_h\) is defined in (25). Assume A1, A2. Then, for any \(r \in (0,1/11]\), any \(z = (x,p) \in T^*M\) and any \(h \in (0, h_1(\|p\|_{g(x)^{-1}}, r, \alpha))\), there exists a unique \(z' \in B_{\|z\|}(z, r) \subset T^*M\) such that \(z' \in G_h(z)\).

**Proof.** Assume A1, A2. Let \(r \in (0,1/11]\), \(z = (x,p) \in T^*M\) and \(h \in (0, h_1(\|p\|_{g(x)^{-1}}, r, \alpha))\), where \(h_1\) is defined in (45). We recall that the map \(g_h\) is defined in (26). We define \(B = B_{\|z\|}(z, r)\) and the map \(g_{h,z} : T^*M \to \mathbb{R}^n \times \mathbb{R}^n\) by \(g_{h,z}(z') = z' - g_h(z, z')\) for any \(z' \in T^*M\). Then, \(g_{h,z}(z') = z'\) if and only if \(z' \in G_h(z)\). The proof is divided in two steps.

**Step 1.** We first prove that \(g_{h,z}(B) \subset B\). Let \(z' \in B\), we have by Lemma 12-(a)
\[
g_{h,z}(z') - z\|_z = \frac{1}{2}\|\{g(x)^{-1} + (g'(x)^{-1})\}p\|_{g(x)} + \frac{1}{4}\|Dg(x)\|_{g(x)}\|g'(x)^{-1}p\|_{g(x)} + \frac{1}{4}\|Dg(x)\|_{g(x)}\|g'(x)^{-1}p\|_{g(x)},
\]
\[
\leq \frac{1}{2}(2\|p\|_{g(x)^{-1}} + \|g(x)^{1/2}(g'(x)^{-1} - g(x)^{-1})g(x)^{1/2}\|_{g(x)^{-1}}\|p\|_{g(x)^{-1}}) + \frac{1}{4}\|p\|_{g(x)^{-1}}^2,
\]
where the following inequalities hold
\[(a)\] \(\|p\|_{g(x)^{-1}} = \|p' - p + p\|_{g(x)^{-1}} \leq r + \|p\|_{g(x)^{-1}}.\]
\[(b)\] \(\|g(x)^{1/2}(g'(x)^{-1} - g(x)^{-1})g(x)^{1/2}\|_2 \leq 3\|x - x'\|_{g(x)} \leq 3r\), on the model of (14), using \(r \leq 1/11\).

Therefore, we have
\[
g_{h,z}(z') - z\|_z \leq h((r + \|p\|_{g(x)^{-1}}) + \frac{3}{2}r(r + \|p\|_{g(x)^{-1}}) + \frac{1}{2}(r + \|p\|_{g(x)^{-1}})^2)
\]
\[
\leq h(r + \|p\|_{g(x)^{-1}})(1 + \frac{3}{2}r) + \frac{1}{2}(r + \|p\|_{g(x)^{-1}})^2
\]
\[
\leq hr/h_1(\|p\|_{g(x)^{-1}}, r, \alpha) < r,
\]
which proves the statement.
Step 2. We now prove that \( g_{h,z} \) is a contraction on \( B \). This proof notably recovers some elements of the proof of Proposition 2 (see Appendix D). Let \((z_1, z_2) \in B \times B \) with \( z_1 = (x_1, p_1) \) and \( z_2 = (x_2, p_2) \). Remark that \( x_1, x_2 \in W^0(x, 1) \times W^0(x, 1) \). Let us first bound \( \| g^{(1)}_{h_1, z_1}(z_1) - g^{(1)}_{h_2, z_2}(z_2) \|_{g(x)} \). We have

\[
\| g^{(1)}_{h_1, z_1}(z_1) - g^{(1)}_{h_2, z_2}(z_2) \|_{g(x)} = \frac{h}{2} \{ g(x)^{-1}(p_1 - p_2) + g(x)^{-1}p_1 - g(x)^{-1}p_2 \}
\]

and then, since \( r \leq 1/11 \), we have on the model of (14)

\[
\| g^{(1)}_{h_1, z_1}(z_1) - g^{(1)}_{h_2, z_2}(z_2) \|_{g(x)} \leq \frac{h}{2} \{ 1 + \| g(x) \|_1 \} \| p_1 - p_2 \|_{g(x)}^{-1} \]

Let us now bound \( \| g^{(2)}_{h_1, z_1}(z_1) - g^{(2)}_{h_1, z_2}(z_2) \|_{g(x)}^{-1} \). We have

\[
\| g^{(2)}_{h_1, z_1}(z_1) - g^{(2)}_{h_1, z_2}(z_2) \|_{g(x)}^{-1} = \frac{h}{2} \{ Dg(x)[g(x)^{-1}p_1, g(x)^{-1}p_1] - Dg(x)[g(x)^{-1}p_2, g(x)^{-1}p_2] \}
\]

which gives using Lemma 12-(a)

\[
\| g^{(2)}_{h_1, z_1}(z_1) - g^{(2)}_{h_1, z_2}(z_2) \|_{g(x)}^{-1} \leq \frac{h}{2} \| Dg(x)[g(x)^{-1}p_1, g(x)^{-1}p_2] \|_{g(x)}^{-1} \]

Finally, it comes that

\[
\| g_{h_1, z_1}(z_1) - g_{h_1, z_2}(z_2) \| \leq \frac{h}{2} \{ 1 + (1 - r)^{-2} + 4r + 2\| p \|_{g(x)}^{-1} \} \| p_1 - p_2 \|_{g(x)}^{-1} \]

which proves that \( g_{h_1, z} \) is a contraction on \( B \).

Conclusion. We obtain the result of Lemma 23 by applying the fixed point theorem on \( g_{h_1, z} \) and \( B \).

Elaborating on Lemma 23, we prove in Lemma 24 that the only element of \( G_h(z^{(0)}) \) verifies smoothness properties if \( h \) is chosen small enough, depending on \( z^{(0)} \).

**Lemma 24.** For any \( z = (x, p) \in T^* M \), any \( r \in (0, 1) \) and any \( \alpha \geq 1 \), we define

\[
\hat{h}(z, r, \alpha) = \min \{ h_1(\| p \|_{g(x)}^{-1}, r, \alpha), h_2(z), h_3(z, r) \}
\]

(46)

where \( h_1 \) is defined in (45), and \( h_2 \) and \( h_3 \) are defined by

\[
h_2(z) = \frac{1}{3/2 + 3\| p \|_{g(x)}^{-1}}, \quad h_3(z, r) = \frac{1}{1 + (1 - r)^{-1}(r + \| p \|_{g(x)}^{-1})}.
\]

We recall that \( r^* \) is defined in (29). We also recall that the maps \( G_h, g_{h}, \overline{G}_h \) and \( G_{h, z^{(0)}} \) are respectively defined in (25), (26), (27) and (28). Assume A1, A2. Then, for any \( z^{(0)} \in T^* M \) and any \( h \in (0, \hat{h}(z^{(0)}, r^*, \alpha)) \), there exists a unique element \( z^{(1/2)}_h = G_h(z^{(0)}) \cap B_{\| x \|_{g(x)}}(z^{(0)}, r^*_{\alpha}) \). Moreover, we have

(a) \( \text{Jac}_z[G_h](z^{(0)}, z^{(1/2)}_h) \) and \( \text{Jac}[^G_h](z^{(1/2)}_h) \) are invertible,
(b) \( \text{Jac}[G_{h,z(0)}](x_h^{(1/2)}) \) is invertible.

**Proof.** Assume A1, A2. Let \( z^{(0)} \in T^*M \) and \( h \in (0, \bar{h}(z^{(0)}, r^*_h, \alpha)) \), where \( \bar{h} \) is defined in (46). Since \( r^*_h \leq 1/11 \), Lemma 23 ensures the existence and uniqueness of \( z_h^{(1/2)} = (x_h^{(1/2)}, p_h^{(1/2)}) \in T^*M \) such that \( z_h^{(1/2)} = G_{h,z^{(0)}}(z_h^{(1/2)}) \) and \( \| \cdot \|_{r^*_h} \). Moreover, we have \( x_h^{(1/2)} \in \mathcal{W}(x^{(0)}, r^*_h) \), and thus \( \text{Jac}[G_{h,z^{(0)}}](x_h^{(1/2)}) \) is invertible by Lemma 22. Let us prove that \( \text{Jac}_z[g_h](z^{(0)}, z_h^{(1/2)}) \) and \( \text{Jac}[\overline{G}_h](z_h^{(1/2)}) \) are invertible.

**Invertibility of \( \text{Jac}_z[g_h](z^{(0)}, z_h^{(1/2)}) \).** We first remark that \( \text{Jac}_z[g_h](z^{(0)}, z_h^{(1/2)}) = \text{Jac}[\psi_{0,h}](z_h^{(1/2)}) \) where \( \psi_{0,h} = \text{Id} + \frac{1}{2} \psi_0 \) and \( \psi_0 \) is defined on \( T^*M \) by

\[
\psi_0(z) = (-g(x^{(0)})^{-1} + g(y)^{-1})^{-1}p - \frac{1}{2} Dg(x^{(0)})[g(x^{(0)})^{-1}p, g(x^{(0)})^{-1}p]).
\]

We recall that \( \|z_h^{(1/2)} - z^{(0)}\|_{z(0)} \leq r^*_h \leq 1/11 \) and thus define \( r_1 = 1/11 - \|z_h^{(1/2)} - z^{(0)}\|_{z(0)} > 0 \) and \( B_1 = B_{1/11}(z_h^{(1/2)}, r_1) \). We set \( \tilde{r} = 1/11 \). Note that \( B_1 \subset B_{1/11}(z^{(0)}, 1/11) \). We show below that \( \psi_0 \) is Lipschitz-continuous on \( B_1 \) with respect to \( \| \cdot \|_{z(0)} \). Let \( (z, z') \in B_1 \times B_1 \). Similarly to the proof of Lemma 23, we have

\[
\|\psi_0^{(1)}(z) - \psi_0^{(1)}(z')\|_{g(x^{(0)})} \leq \|p - p'\|_{g(x^{(0)})}^{-1} + \|g(x^{(0)})^{1/2}g(x)^{-1}g(x^{(0)})^{1/2}\|_{2}\|p - p'\|_{g(x^{(0)})}^{-1} + \|g(x^{(0)})^{1/2}\{g(x) - g(x')\}g(x^{(0)})^{1/2}\|_{2}\|p\|_{g(x^{(0)})}^{-1}
\]

\[
\leq (1 + (1 - \tilde{r})^{-2})\|p - p'\|_{g(x^{(0)})}^{-1} + 3(1 - \tilde{r})^{-3}(\tilde{r} + \|p(0)\|_{g(x^{(0)})}^{-1})\|x - x'\|_{g(x^{(0)})}^{-1}.
\]

In the same manner, we have

\[
\|\psi_0^{(2)}(z) - \psi_0^{(2)}(z')\|_{g(x^{(0)})} \leq 2(2\tilde{r} + \|p(0)\|_{g(x^{(0)})}^{-1})\|p - p'\|_{g(x^{(0)})}^{-1}.
\]

Therefore, recalling that \( \tilde{r} = 1/11 \), we obtain with the previous inequalities

\[
\|\psi_0(z) - \psi_0(z')\|_{z(0)} \leq \{3 + 6\|p(0)\|_{g(x^{(0)})}^{-1}\}\|z - z'\|_{z(0)} \leq 2\|z - z'\|_{z(0)}/h_2(z^{(0)}).
\]

Hence, \( \psi_0 \) is \( (2/h_2(z^{(0)}))\)-Lipschitz-continuous on \( B_1 \) with respect to \( \| \cdot \|_{z(0)} \). Then, since \( h < h_2(z^{(0)}) \), \( \text{Jac}[\psi_{0,h}](z) \) is invertible for any \( z \in B_1 \) by Lemma 21. In particular, \( \text{Jac}_z[g_h](z^{(0)}, z_h^{(1/2)}) = \text{Jac}[\psi_{0,h}](z_h^{(1/2)}) \) is invertible.

**Invertibility of \( \text{Jac}[\overline{G}_h](z_h^{(1/2)}) \).** Let us remark that \( \overline{G}_h = \text{Id} + h\zeta \) where \( \zeta \) is defined on \( T^*M \) by

\[
\zeta(z) = (0, \frac{1}{4} Dg(x)[g(x)^{-1}p, g(x)^{-1}p]).
\]

We define \( r_2 = 1/2 \) and \( B_2 = B_\|z_h^{(1/2)}\|_{z_h^{(1/2)}}(z_h^{(1/2)}, r_2) \). We show below that \( \zeta \) is Lipschitz-continuous on \( B_2 \) with respect to \( \| \cdot \|_{z_h^{(1/2)}} \), with a Lipschitz constant which does not depend on \( z_h^{(1/2)} \). Let \( (z, z') \in B_2 \times B_2 \). Using Lemma 12-(a) with \( r_2 = 1/2 \), it is clear that

\[
\|\zeta(z) - \zeta(z')\|_{z_h^{(1/2)}} \leq (1 + \|p_h^{(1/2)}\|_{g(x_h^{(1/2)})}^{-1})\|z - z'\|_{z_h^{(1/2)}}.
\]

Moreover, since \( \|z_h^{(1/2)} - z^{(0)}\|_{z(0)} < r^*_h \), we have by Lemma 15

\[
\|p_h^{(1/2)}\|_{g(x_h^{(1/2)})}^{-1} \leq (1 - r^*_h)^{-1}\|p_h^{(1/2)}\|_{g(x^{(0)})}^{-1}.
\]
\[ \leq (1 - r_{\alpha}^*)^{-1}(r_{\alpha}^* + \|p^{(0)}\|_{g_{\xi(x^0) - 1}}) , \]

and thus
\[ \|\xi(z) - \xi(z')\|_{h/2} \leq \{1 + (1 - r_{\alpha}^*)^{-1}(r_{\alpha}^* + \|p^{(0)}\|_{g_{\xi(x^0) - 1}})\}\|z - z'\|_{h/2} \]

\[ \leq \|z - z'\|_{h/2}/h_3(z^{(0)}, r_{\alpha}^*) . \]

Hence, \( \xi \) is \((1/h_3(z^{(0)}, r_{\alpha}^*))\)-Lipschitz-continuous on \( B_2 \) with respect to \( \| \cdot \|_{h/2} \). Since \( h < h_3(z^{(0)}, r_{\alpha}^*) \), \( \text{Jac}[\xi_h](z) \) is invertible for any \( z \in B_2 \) by Lemma 21. In particular, \( \text{Jac}[\xi_h](z^{(1/2)}) \) is invertible, which concludes the proof.

The following lemma states the existence of a diffeomorphism between \( z^{(0)} \in T^*M \) and \( z^{(1)} \in G_h(z^{(0)}) \) under smoothness conditions verified by \( z^{(1)} \).

**Lemma 25.** Let \( (z^{(0)}, z^{(1)}) \in T^*M \times T^*M \). We recall that the maps \( g_h, \overline{G}_h \) and \( G_h \) are respectively defined in (26), (27) and (4). Assume that \( \mathfrak{g} \in C^2(M, \mathbb{R}^{d \times d}) \) and that there exist \( h > 0 \) and \( z_h^{(1/2)} \in T^*M \) with the following properties:

(a) \( g_h(z^{(0)}, z_h^{(1/2)}) = 0 \) and \( z_h^{(1)} = \overline{G}_h(z_h^{(1/2)}) \).

(b) \( \text{Jac}_z[g_h](z^{(0)}, z_h^{(1/2)}) \) and \( \text{Jac}[\overline{G}_h](z_h^{(1/2)}) \) are invertible.

Then, there exists a neighbourhood \( U \subset T^*M \) of \( z^{(0)} \) and a \( C^1 \)-diffeomorphism \( \xi : U \rightarrow \xi(U) \subset T^*M \) such that (i) \( \xi(z^{(0)}) = z^{(1)} \), (ii) for any \( z \in U, \xi(z) \in G_h(z) \) and (iii) \( \det\text{Jac}\xi \equiv 1 \).

**Proof.** Let \( (z^{(0)}, z^{(1)}) \in T^*M \times T^*M \). Assume that \( \mathfrak{g} \in C(M, \mathbb{R}^{d \times d}) \) and consider \( h > 0 \) and \( z_h^{(1/2)} \in T^*M \) as described in Lemma 25. Under the assumption on \( g, g_h \) and \( \overline{G}_h \) are continuously differentiable respectively on \( T^*M \times T^*M \) and \( T^*M \). We are going to prove Lemma 25, by first deriving intermediary results on \( g_h \) and \( \overline{G}_h \).

**Result on \( g_h \).** We recall that \( g_h(z^{(0)}, z_h^{(1/2)}) = 0 \) and \( \text{Jac}_z[g_h](z^{(0)}, z_h^{(1/2)}) \) is invertible. Then, by applying the implicit function theorem on \( g_h \) at \( (z^{(0)}, z_h^{(1/2)}) \), we obtain the existence of a neighbourhood \( U_0 \subset T^*M \) of \( z^{(0)} \) and a \( C^1 \)-diffeomorphism \( \xi_0 : U_0 \rightarrow \xi_0(U_0) \subset T^*M \) such that \( \xi_0(z^{(0)}) = z_h^{(1/2)} \) and for any \( z \in U_0, g_h(z, \xi_0(z)) = 0 \), i.e., \( \xi_0(z) \in \overline{G}_h(z) \). Moreover, for any \( z \in U_0 \), the Jacobian of \( \xi_0 \) at \( z \) is given by
\[ \text{Jac}[\xi_0](z) = -\text{Jac}_z[g_h](z, \xi_0(z))^{-1}\text{Jac}_z[g_h](z, \xi_0(z)) . \]

**Result on \( \overline{G}_h \).** We recall that \( z^{(1)} = \overline{G}_h(z_h^{(1/2)}) \) and \( \text{Jac}[\overline{G}_h](z_h^{(1/2)}) \) is invertible. Then, we apply the inverse function theorem on \( \overline{G}_h \) at \( z_h^{(1/2)} \) and obtain the existence of a neighbourhood \( U_1 \subset T^*M \) of \( z_h^{(1/2)} \) such that \( \xi_1 = \overline{G}_h|_{U_1} \) is a \( C^1 \)-diffeomorphism on \( U_1 \).

**Final result.** We now consider the subset \( U \) and the map \( \xi \), respectively defined by

(a) \( U = \xi_0^{-1}(U_1 \cap \xi_0(U_0)) \subset T^*M \), neighbourhood of \( z^{(0)} \).

(b) \( \xi = \xi_1|_{\xi_0(U)} \circ \xi_0 \), \( C^1 \)-diffeomorphism on \( U \) such that \( \xi(z^{(0)}) = z^{(1)} \), and for any \( z \in U, \xi(z) \in G_h(z) \).

Let us now prove that \( |\det\text{Jac}\xi| \equiv 1 \). Let \( z \in U \). We define \( z_0 = \xi_0(z) \). By the chain rule, we have
\[ \text{Jac}[\xi](z) = \text{Jac}[\xi_1 \circ \xi_0](z) \]
\[ = \text{Jac}[\xi_1](\xi_0(z)) \text{Jac}[\xi_0](z) \]
\[ = -\text{Jac}[\xi_1](\xi_0(z)) \text{Jac}_z[g_h](z, \xi_0(z))^{-1}\text{Jac}_z[g_h](z, \xi_0(z)) , \]

where we have
Lemma 26. Let \( h > 0 \). We recall that the set-valued map \( F_h \) is defined in Section 4.1. Let \( z \in T^*M \). Assume that there exist \( (z', z'') \in T^*M \times T^*M \) such that (i) \( z' \in F_h(z) \), (ii) \( z'' \in F_h(z) \), and (iii) \( x' = x'' \). Then, we have \( p' = p'' \), and thus \( z' = z'' \).

Proof. Let \( h > 0 \). Let \( z \in T^*M \). We consider \( (z', z'') \in F_h(z) \) \times \( F_h(z) \) such that \( x' = x'' = \hat{x} \). By using the last two equations from (4) with \( z' \) and \( z'' \), we have \( p' = -p^{(1/2)} + \frac{\hat{h}(\hat{x})^{−1}}{2} p^{(1/2)} = p'' \), where \( p^{(1/2)} = \frac{\hat{h}}{h}(\hat{x})^{−1} + \hat{g}(\hat{x})^{−1}−1(\hat{x} - x) \), which concludes the proof.

Under the assumption A2, we define, for any \( z^{(0)} \in T^*M \), \( h^*(z^{(0)}) = \hat{h}(s(z^{(0)}), r^*_n, \alpha) \), where \( \alpha \) is given by A2, and \( r^*_n \) and \( \hat{h} \) respectively defined in (29) and (46). Note that \( h^* \) appears in Proposition 5, for which we derive the proof below.

Proof of Proposition 5. We recall that maps \( \mathcal{G}_h \), \( \mathcal{E}_h \) and \( \mathcal{C}_h \) are respectively defined in (25), (26) and (27). Assume A1, A2. Let \( z^{(0)} \in T^*M \). We define \( \hat{z}^{(0)} = s(z^{(0)}) \). Let \( h \in (0, h^*(z^{(0)})) \). By using Lemma 24 on \( \hat{z}^{(0)} \), we obtain the existence of \( z^{(1/2)}(z^{(0)}) \in T^*M \) with the following properties:

(a) \( z^{(1/2)} \in \mathcal{C}_h(\hat{z}^{(0)}) \), i.e., \( \mathcal{E}_h(\hat{z}^{(0)}) \times \mathcal{G}_h(z^{(0)}) = 0 \),
(b) \( \text{Jac}(\mathcal{E}_h)(z^{(0)}) \) and \( \text{Jac}(\mathcal{G}_h)(z^{(1/2)}) \) are invertible,
(c) \( \text{Jac}(\mathcal{G}_h)(z^{(1/2)}) \) is invertible.

We then define \( z^{(1)} = \mathcal{C}_h(z^{(1/2)}) \). In particular, \( z^{(1)} \in \mathcal{G}_h(z^{(0)}) \), i.e., \( z^{(1)} \in F_h(z^{(0)}) \) and \( \text{Jac}(\mathcal{G}_h)(z^{(1)} = \text{Jac}(\mathcal{G}_h)(z^{(1/2)}) ) \) is invertible. By combining the properties of \( z^{(1/2)} \) and with Lemma 25, we also obtain the existence of a neighbourhood \( U' \subset T^*M \) of \( \hat{z}^{(0)} \) and a \( C^1 \)-diffeomorphism \( \xi_h : U' \to \xi_h(U') \subset T^*M \) such that (i) \( \xi_h(\hat{z}^{(0)}) = z^{(1)} \),
(ii) for any \( z \in U' \), \( \xi_h(z) \in \mathcal{G}_h(z) \) and (iii) \( \det \text{Jac} \xi_h \equiv 1 \). Therefore, we can define the subset \( U \) and the map \( \gamma_h \) of Proposition 5 by

(a) \( U = s(U') \), neighbourhood of \( z^{(0)} \) in \( T^*M \),
(b) \( \gamma_h = \xi_h \circ s \), such that (i) \( \gamma_h(z^{(0)}) = z^{(1)} \), (ii) for any \( z \in U \), \( \gamma_h(z) \in F_h(z) \) and (iii) \( \det \text{Jac}[\gamma_h] \equiv 1 \).

We now prove that \( U \) can be reduced to a smaller subset such that \( \gamma_h(z) \) is the only element of \( F_h(z) \) in \( \gamma_h(U) \) for any \( z \in U \). Motivated by Lemma 22, we first define, for any \( (x, x') \in M \times M \), \( F_{h,x}(x') \) as the only element \( p \in T^*_xM \) such that \( (x', p') \in F_h(x, p) \) for any \( p' \in T^*_xM \). It is clear that \( F_{h,x}(x') = -G_{h,x}(x') \), where \( G_{h,x} \) is defined in (28). We also define \( Z_h : M \times M \to T^*M \) by

\[
Z_h(x, x') = (x, F_{h,x}(x')) = (x, -G_{h,x}(x'))
\]

which is continuously differentiable since \( g \in C^2(M, \mathbb{R}^{d \times d}) \). Besides this, by Lemma 22, \( \text{Jac}(\mathcal{G}_h(0))(x^{(0)}, x^{(1)}) \) is invertible, and then \( \text{Jac}(Z_h)(x^{(1)}) \) is invertible. Therefore, by applying the inverse function theorem on \( Z_h \) at \((x^{(0)}, x^{(1)})\),
it comes that $Z_h$ is a $C^1$-diffeomorphism in a neighbourhood of $(x^{(0)}, x^{(1)}_h)$. We are now going to prove the result by contradiction. Assume for now that there is no neighbourhood $U$ of $z^{(0)}$ such that $\gamma_h(z)$ is the only element of $F_h(z)$ in $\gamma_h(U)$, for any $z \in U$. Then, we can find a sequence $(z_i)_{i \in \mathbb{N}}$ which converges to $z^{(0)}$ such that for any $i \in \mathbb{N}$, there exist two different elements $z_{i,1} \in F_h(z_i)$ and $z_{i,2} \in F_h(z_i)$. Therefore, for any $i \in \mathbb{N}$, $x_{i,1} \neq x_{i,2}$ and by Lemma 26, we have

$$F_{h,x_i}(x_{i,1}) = F_{h,x_i}(x_{i,2}) = p_i,$$

and thus

$$Z_h(x_i, x_{i,1}) = Z_h(x_i, x_{i,2}) = z_i. \quad (47)$$

Moreover, by continuity of $\gamma_h$, the sequences $(z_{i,1})_{i \in \mathbb{N}}$ and $(z_{i,2})_{i \in \mathbb{N}}$ converge to $z^{(1)}_h$, and therefore, $(x_{i,1})_{i \in \mathbb{N}}$ and $(x_{i,2})_{i \in \mathbb{N}}$ also converge to $x^{(1)}$. Combined with (47), this result of convergence is in contradiction with the fact that $Z_h$ is a diffeomorphism in a neighbourhood of $(x^{(0)}, x^{(1)}_h)$. Therefore, we can reduce $U$ to a smaller subset such that $\gamma_h(z)$ is the only element of $F_h(z)$ in $\gamma_h(U)$ for any $z \in U$, which concludes the proof of Proposition 5. □

G Modification of n-BHMC algorithm with step-size conditioning

In the rest of the paper, for any $z^{(0)} \in T^*M$, we will denote by $h_*(z^{(0)})$ the value of $h_*$ given by A3.

Beyond n-BHMC. A crucial part of the proof of reversibility in BHMC, as much for c-BHMC as for n-BHMC, relies on local symplectic properties of the integrator of the Hamiltonian dynamics. Although Algorithm 2 can be implemented without any practical limitation, it is hard to state such properties for its numerical integrator $\Phi_h$ under A1, A2 and A3, given any value of $h$. Indeed, we know from A3 that $\Phi_h$ is a local involution around $z^{(0)} \in T^*M$ when $h < h_*(z^{(0)})$; however, we cannot ensure this result when $h > h_*(z^{(0)})$. To circumvent this issue, we propose to study Theoretical n-BHMC (Tn-BHMC), presented in Algorithm 3. In this modified version of n-BHMC, we actually enforce a condition on $h$ to be small enough. We now get into the details of this new algorithm and assume A3 for the rest of this section.

Theoretical motivations. Let $h > 0$. Using notation from A3, we define

$$A_h = \{ z \in T^*M : h < \min_{\tilde{z} \in B_{1,h}(z^{(1)})} h_*(\tilde{z}) \}.$$

It is clear that $A_h \subset \text{dom}_{\Phi_h}$; indeed, if $z^{(0)} \in A_h$, we have in particular that $h < h_*(z^{(0)})$, and therefore $z^{(0)} \in \text{dom}_{\Phi_h}$ by A3. Let $z^{(0)} \in A_h$. We can properly define $z^{(1)} = \Phi_h(z^{(0)})$. By A3, we know that $\Phi_h$ is an involution on a neighbourhood of $z^{(0)}$; in particular, it comes that $(\Phi_h \circ \Phi_h)(z^{(0)}) = z^{(0)}$, i.e., $\Phi_h(z^{(1)}) = z^{(0)}$. Hence, if $z^{(0)} \in A_h$, the "reverse integration check" of Step 2 in Algorithm 2 is always true. This simple analysis of $A_h$ motivates us to replace the condition of belonging to $\text{dom}_{\Phi_h}$ by the condition of belonging to $A_h$.

Implementation of Tn-BHMC. In Algorithm 3, we highlight in yellow the modifications of Tn-BHMC in contrast to n-BHMC. Namely, we replace

(a) "$z^{(0)} \in \text{dom}_{\Phi_h}$" (Line 10 in Algorithm 2) by "$z^{(0)} \in A_h$" (Line 10 in Algorithm 3).

(b) "$z^{(1)} \in \text{dom}_{\Phi_h}$" (Line 14 in Algorithm 2) by "$z^{(1)} \in A_h$" (Line 12 in Algorithm 3).

Note that there is no need to maintain the "reverse integration check" of Algorithm 2, since it is automatically verified once $z^{(0)} \in A_h$. On the whole, these new conditions are more restrictive than the conditions of Algorithm 2 since $A_h \subset \text{dom}_{\Phi_h}$; moreover, they can be thought as conditions directly applied on the step-size $h$. The specific choice of $A_h$, instead of another subset of $\text{dom}_{\Phi_h}$, is actually sufficient to derive the proof of reversibility of Tn-BHMC (see Section 5.2).
Algorithm 3 Tn-BHMC with Momentum Refreshment

1: HMC Input: \((x_0, p_0) \in T^* M, \beta \in (0, 1], N \in \mathbb{N}\)
2: ODE Input: \(h, \eta, \Phi_h, A_h\)
3: Output: \((x_n, p_n)_{n \in [N]}\)
4: for \(t = 1, ..., N\) do
5: \(x, p \leftarrow x_{n-1}, p_{n-1}\)
6: Step 1: \(\tilde{p} \sim N_x(0, \text{Id})\), \(\bar{p} \sim \sqrt{1 - \beta}p + \sqrt{\beta} \tilde{p}\)
7: Step 2: solving discretized ODE (3)
8: \(\bar{x}', \bar{p}' \leftarrow x, p\)
9: \(x^{(0)}, p^{(0)} \leftarrow (s \circ S_{h/2})(x, p)\)
10: if \(\bar{x}^{(0)} \in A_h\) then
11: \(z^{(1)} = \Phi_h(z^{(0)})\)
12: if \(\bar{x}^{(1)} \in A_h\) then
13: \(\bar{x}', \bar{p}' \leftarrow (s \circ S_{h/2})(x^{(1)}, p^{(1)})\)
14: Step 3: \(\alpha \leftarrow \min(1, \exp[-H(x', p') + H(x, p)])\)
15: \(u \sim U[0, 1]\)
16: if \(u \leq \alpha\) then
17: \(\bar{x}_n, \bar{p}_n \leftarrow x', p'\)
18: else
19: \(\bar{x}_n, \bar{p}_n \leftarrow x, p\)
20: Step 4: \(x_n, p_n \leftarrow s(x_t, \bar{p}_t)\)
21: Step 5: \(\tilde{p} \sim N_x(0, \text{Id})\), \(p_n \leftarrow \sqrt{1 - \beta}p_n + \sqrt{\beta} \tilde{p}\)

H Proofs of Section 5.2

H.1 Expression and properties of \(r^*\)

Given a Riemannian manifold \((M, \mathfrak{g})\), we define \(r^*(x)\), or equivalently \(r^*_x\), for any \(x \in M\) by

\[
r^*(x) = \min(\|g(x)\|^{-1/2}, \|g(x)^{-1}\|^{-1/2}) \, .
\]  (48)

Note that \(r^*\) is used in A3 and that \(r^*(x) = 1/C_x\), where \(C_x\) is defined in Lemma 15. We prove below that \(r^*\) has a smooth behaviour on \(M\) under our main assumptions.

Lemma 27. Assume A1, A2. Also assume that \(x \in M \mapsto \|g^{-1}(x)\|_2\) is bounded from above. As defined in (48), \(r^* : M \to (0, +\infty)\) satisfies the following properties:

(a) \(r^*(x) \to 0\) as \(x \to \partial M\).
(b) There exists \(L > 0\) such that \(r^*\) is \(L\)-Lipschitz-continuous on \(M\) with respect to \(\|\cdot\|_2\).
(c) There exists \(M > 0\) such that \(r^*(x) \leq M\) for any \(x \in M\).

Proof. Assume A1, A2. Also assume that \(x \in M \mapsto \|g^{-1}(x)\|_2\) is bounded from above. We first define \(r_1 : x \in M \mapsto \|g(x)\|_2^{-1/2}\) and \(r_2 : x \in M \mapsto \|g(x)^{-1}\|^{-1/2}_2\), such that \(r^* = \min(r_1, r_2)\). Since \(g \in C^2(M, \mathbb{R}^{d \times d})\), it is clear that \(r_1\) and \(r_2\) are continuously differentiable on \(M\). We have: (i) \(r_1(x) \to 0\) as \(x \to \partial M\) by Lemma 11, and (ii) \(r_2(x) \to 0\) as \(x \to \partial M\), since \(1/r_2^2 : x \mapsto \|g(x)^{-1}\|^{-2}_2\) is bounded on \(M\). Combining the fact that \(r_2(x) > 0\) for any \(x \in M\) and item (i), we obtain item (a) of Lemma 27.

We denote by \(d\) the distance induced by \(\|\cdot\|_2\) and now define, for any \(\varepsilon > 0\),

(a) \(\mu_\varepsilon = \inf_{y \in M : d(y, \partial M) \leq \varepsilon} r_2(y)\).
(b) $M_\varepsilon = \text{Int}(\{x \in M : d(x, \partial M) \leq \varepsilon, r_1(x) \leq \mu_\varepsilon\})$, open set in $M$.
(c) $M_{-\varepsilon} = M \setminus M_\varepsilon$, closed and bounded (and thus, compact) set in $M$.

Using items (i) and (ii), we can ensure the existence of some $\varepsilon \in (0, \text{diam}(M))$ such that (i) $\mu_\varepsilon > 0$ and (ii) $M_\varepsilon$ and $M_{-\varepsilon}$ are not empty. We consider such $\varepsilon$ for the rest of the proof.

**Smoothness of $r_2$.** We define $\delta = d(M^c, M_{-\varepsilon})$ and $M_\delta = M^c + B(0, \delta/4)$. Note that (i) $\delta > 0$ since $M_{-\varepsilon} \subset M$, (ii) $M_\delta$ is closed since the ball $B(0, \delta/4)$ is compact, and (iii) $M_\delta \cap M_{-\varepsilon} = \emptyset$. According to the smooth version Urysohn’s lemma applied to $M_\delta$ and $M_{-\varepsilon}$, there exists $\chi \in C^4([0, 1])$ such that $\chi(M_{-\varepsilon}) = 1$ and $\chi(M_\delta) = 0$. We then define $\tilde{r}_2 : \mathbb{R}^d \to (0, +\infty)$ by $\tilde{r}_2 = \chi r_2 + (1 - \chi)\mu_\varepsilon$. In particular, (i) there exists $L_2 > 0$ such that $\tilde{r}_2$ is $L_2$-Lipschitz-continuous on $M$ with respect to $\|\cdot\|_2$, since $\tilde{r}_2 \in C^1([0, 1])$, and (ii) for any $x \in M_\varepsilon$, $\tilde{r}_2(x) > \mu_\varepsilon$.

**Smoothness of $r_1$.** We now prove that $r_1$ is $1$-Lipschitz continuous on $M$ with respect to $\|\cdot\|_2$. Let $x \in M$. Note that $r_1(x) = (\|g(x)\|_2^2)^{-1/4}$ and we thus have

$$
\nabla r_1(x) = (-1/4)\|g(x)\|_2^{-5/2} h(x) : Dg(x),
$$

where $h(x) = \partial g(x)\|g(x)\|_2^2 = 2\|g(x)\|_2 u(x) u(x)^T$, $u(x)$ being a normal eigenvector of $g(x)$ corresponding to the eigenvalue $\|g(x)\|_2$. Hence,

$$
\|\nabla r_1(x)\|_2 \leq (1/2)\|g(x)\|_2^{-3/2}\|u(x)u(x)^T : Dg(x)\|_2 \leq (1/2)\|g(x)\|_2^{-3/2}\|u(x)u(x)^T\|_2\|Dg(x)\|_2 \
\leq (1/2)\|g(x)\|_2^{-3/2} \times 2\|g(x)\|_2^{3/2} \leq 1
$$

(Definition 1-(c))

which proves the result on $r_1$.

**Smoothness of $r$.** Let $x \in M$. We can face two cases: either, $x \in M_{-\varepsilon}$, then $r_2(x) = \tilde{r}_2(x)$; or, $x \in M_\varepsilon$, then $\tilde{r}_2(x) > \mu_\varepsilon \geq r_1(x)$ and $r_2(x) \geq r_1(x)$ by definition of $M_\varepsilon$. Thus, we have for any $x \in M$, $r_2(x) = \min(r_1(x), \tilde{r}_2(x))$ where $r_1$ and $\tilde{r}_2$ are respectively $1$ and $L_2$ Lipschitz-continuous on $M$ with respect to $\|\cdot\|_2$. By observing that $2\min(r_1, \tilde{r}_2) = r_1 + \tilde{r}_2 - |r_1 - \tilde{r}_2|$, we set $L = 1 + L_2$ and thus obtain item (b) of Lemma 27. Finally, item (c) of Lemma 27 directly derives from item (b), since $M$ is bounded.

Note that the extra-assumption on $g^{-1}$ used in Lemma 27 is not directly ensured by self-concordance but can be proved when $M$ is a polytope, as shown below.

**Lemma 28.** Consider a polytope $M$ defined by $m$ constraints with $m > d$ such that $M = \{x : Ax < b\}$, where $A \in \mathbb{R}^{m \times d}$ is a full-rank matrix and $b \in \mathbb{R}^m$. We endow $M$ with the Riemannian metric $g(x) = D^2\phi(x)$ where $\phi : M \to \mathbb{R}$ is the logarithmic barrier given for any $x \in M$ by $\phi(x) = -\sum_{i=1}^m \ln(b_i - A_i^T x)$. In particular, $M$ and $g$ verify A1 and A2. Then, the function $r : M \to (0, +\infty)$ defined by $r(x) = \|g^{-1}(x)\|_2$, for any $x \in M$, is bounded from above.

**Proof.** Consider such manifold $M$ and metric $g$. We aim to show that the smallest eigenvalue of $g(x)$ is bounded from below for any $x \in M$ by a constant $c > 0$, which does not depend on $x$, i.e., for any $h \in \mathbb{R}^d$ and any $x \in M$, $g(x)[h, h] \geq c\|h\|_2^2$.

Since $A$ is full-ranked, $A^T A$ is positive-definite. In particular, for any $h \in \mathbb{R}^d$, $(A^T A)[h, h] \geq \lambda_{\min}(A^T A)\|h\|_2^2$, where $\lambda_{\min}(A^T A) > 0$ is the smallest eigenvalue of $A^T A$. We recall that we have for any $x \in M$, $g(x) = A^T S(x)^{-2} A$, where $S(x) = \text{Diag}(b_i - A_i^T x)_{i \in [m]}$. Let $i \in [m]$. The function $r_i : x \in M \mapsto S(x)^{-1/2}_{i,i}$ has the following properties: (i) $r_i$ is continuous on $M$, (ii) $r_i(x) > 0$ for any $x \in M$ and (iii) $r_i(x) \to +\infty$ as $x \to \partial M$. Thus, there exists $c_i > 0$ such that for any $x \in M$, $r_i(x) \geq c_i$. We define $\tilde{c} = \min_{i \in [m]} c_i$ and we have for any $x \in M$, $S(x)^{-2} \geq \tilde{c} I_d$. We now define $c = \tilde{c} \lambda_{\min}(A^T A)$ and we have for any $x \in M$

$$
g(x)[h, h] \geq \tilde{c} \cdot (A^T A)[h, h] \geq c\|h\|_2^2.
$$

In particular, $g(x)^{-1} \preceq (1/c) I_d$, i.e., $\|g(x)^{-1}\|_2 \leq (1/c)$, which concludes the proof.

□
H.2 Markov kernels of Algorithm 2

Based on the model of $\tilde{E}_h$ defined in (20), we define the set $\tilde{E}_h^\phi \subset T^*M$, which will ensure that the maps derived from implicit integrators of n-BHMC are properly expressed

$\tilde{E}_h^\phi = (s \circ S_{h/2})^{-1}(\text{dom } \Phi_h \cap \Phi_h^{-1}(\text{dom } \Phi_h)) = (s \circ S_{h/2})(\text{dom } \Phi_h \cap \Phi_h^{-1}(\text{dom } \Phi_h))$.

For any $(z, z') \in \tilde{E}_h^\phi \times T^*M$, we define the acceptance probability $\bar{a}(z'|z)$ to move from $z$ to $z'$ by

$\bar{a}(z'|z) = a(z'|z)I(\Phi_h s_{\text{std}}(\phi_h \circ \Phi_h s_{\text{std}}(z)) \in \text{dom } \Phi_h)$,

where $a(z'|z)$ is the acceptance probability defined in (6).

We denote by $Q_n : T^*M \times B(T^*M) \to [0, 1]$, the transition kernel of the (homogeneous) Markov chain $(x_n, p_n)_{n \in [N]}$ generated by Algorithm 2. We also denote by:

(a) $Q_0 : T^*M \times B(T^*M) \to [0, 1]$, the transition kernel referring to Step 1 (also Step 5) in Algorithm 2, defined in (21).

(b) $Q_{n,1} : T^*M \times B(T^*M) \to [0, 1]$, the transition kernel referring to Step 2-3-4 in Algorithm 2.

We provide below details on Markov kernels $Q_n$ and $Q_{n,1}$.

**Kernel $Q_{n,1}$.** This kernel is deterministic and corresponds to the numerical integration of the Hamiltonian up until time $h$. For any $(z, z') \in T^*M \times T^*M$, we have

$Q_{n,1}(z, dz') = \mathbb{I}_{E_h^\phi}(z)(s\# Q_{n,2})(z, dz') + \mathbb{I}_{E_h^\phi}(z)\delta_{s(z)}(dz')$.

where

$q_{n,2}(z, dz') = \bar{a}(R_h^\phi(z) | z)\delta_{R_h^\phi(z)}(dz') + [1 - \bar{a}(R_h^\phi(z) | z)]\delta_{z}(dz')$.

**Kernel $Q_n$.** This kernel corresponds to one step of Algorithm 2 (i.e., comprising Steps 1 to 5). For any $(z, z') \in T^*M \times T^*M$, we have

$Q_n(z, dz') = \int_{T^*M \times T^*M} Q_0(z, dz_1)Q_{n,1}(z_1, dz_2)Q_0(z_2, dz')$.

H.3 Proof of reversibility in Algorithm 3

Let $h > 0$. Using notation from A3, we recall that we defined in Appendix G the set $A_h$ by

$A_h = \{ z \in T^*M : h < \min_{z \in B_{\|z\|}} h_s(\tilde{z}) \subset \text{dom } \Phi_h \}$.

We also recall that $\bar{\pi}$, as defined in (2), admits a density with respect to the product Lebesgue measure given for any $z = (x, p) \in T^*M$ by

$$(d\bar{\pi}/(dx dp))(x, p) = (1/Z) \exp[-(1/2)\|p\|^2_{\tilde{g}(x)} - 1] \det(\tilde{g}(x))^{-1/2} \exp[-V(x)].$$

Since Algorithm 3 can be thought as a restrictive version of Algorithm 2, the Markov kernels from n-BHMC are similar to the kernels from n-BHMC, defined in Appendix H.2. In particular, the transition kernel corresponding to the Gaussian momentum update (Step 1 and 5 in Algorithm 3, Step 1 and 5 in Algorithm 2) is the same and is reversible (up to momentum reversal) with respect to $\bar{\pi}$ (see Lemma 17). Namely, we replace

(a) the set $\tilde{E}_h^\phi$, defined in (49), by $\tilde{E}_h^\phi$,

(b) the kernels $Q_{n,1}$ and $Q_{n,2}$, respectively defined in (50) and (51), by $Q_1$ and $Q_2$, where

$\tilde{E}_h^\phi = (s \circ S_{h/2})^{-1}(A_h \cap \Phi_h^{-1}(A_h)) = (s \circ S_{h/2})(A_h \cap \Phi_h^{-1}(A_h))$,

$Q_1(z, dz') = \mathbb{I}_{E_h^\phi}(z)(s\# Q_2)(z, dz') + \mathbb{I}_{E_h^\phi}(z)\delta_{s(z)}(dz')$,

$Q_2(z, dz') = a(R_h^\phi(z) | z)\delta_{R_h^\phi}(dz') + [1 - a(R_h^\phi(z) | z)]\delta_{z}(dz')$. 

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We denote by $Q : T^*M \times \mathcal{B}(T^*M) \to [0, 1]$, the transition kernel of the (homogeneous) Markov chain $(x_n, p_n)_{n \in [N]}$ generated by Algorithm 3. For any $(z, z') \in T^*M \times T^*M$, we have

$$Q(z, dz') = \int_{T^*M \times T^*M} Q_0(z, dz_1)Q_1(z_1, dz_2)Q_0(z_2, dz').$$

We first turn to the reversibility up to momentum reversal of $Q_1$ with respect to $\bar{\pi}$. We start with the following lemma which is key to establish this result.

**Lemma 29.** Assume A1, A2, A3. Then, for any compact set $G \subset T^*M$, for any $g \in C(T^*M \times T^*M, \mathbb{R})$ such that $\text{supp}(g) \subset G \times G$, we have

$$\int_{G_n} g(z, \Phi_h(z))dz = \int_{G_n} g(\Phi_h(z), z)dz,$$

where $G_n = F_h \cap G \cap \Phi_h^{-1}(G), F_h = A_h \cap \Phi_h^{-1}(A_h), A_h$ being defined in (52).

**Proof.** Assume A1, A2, A3. Let $G \subset T^*M$ be a compact set, $g \in C(T^*M \times T^*M, \mathbb{R})$ such that $\text{supp}(g) \subset G \times G$. We first define the sets $F_h = A_h \cap \Phi_h^{-1}(A_h), G_h = F_h \cap G \cap \Phi_h^{-1}(G)$ and the integrals $I'$ and $J'$

$$I' = \int_{G_n} g(z, \Phi_h(z))dz, \quad J' = \int_{G_n} g(\Phi_h(z), z)dz.$$

We recall the existence under A1 and A2 of $L > 0$ and $N > 0$ such that $r^*$, given by A3 and defined in (48), is $L$-Lipschitz-continuous on $M$ with respect to $\| \cdot \|_2$ and bounded from above by $H$ (see Lemma 27).

We define $r : T^*M \to (0, +\infty)$ by $r(x, p) = r^*(x)/m$ for any $(x, p) \in T^*M$, where $m = \max \{1/\lambda, 4M, 4L\}$ and $\lambda$ is given by A3. Using the properties of $r^*$, it comes that (a) $r$ is $L$-Lipschitz on $T^*M$ with respect to $\| \cdot \|_2$, (b) $r(x, p) \leq 1/(4LCZ)$ for any $(x, p) \in T^*M$, where $C_Z$ is defined in Lemma 15, (c) $r \leq 1/4$, and (d) $r \leq \lambda r^*$.

Note that $G \subset \cup_{i \in [K]} B_{\|\|_\lambda}(z, r(z)).$ Since $G$ is a compact set, there exist $K \in \mathbb{N}$ and $(z_i)_{i \in [K]} \subset T^*M^K$ such that $G \subset \cup_{i=1}^K B_{\|\|_\lambda}(z_i, r(z))$. We consider the sequence $\{V_i\}_{i=1}^K$ constructed as follows: $V_1 = G \cap B_1$ and for any $i \in \{2, \ldots, K\}$, $V_i = (G \cap B_i) \cap (\cup_{j=1}^{i-1} V_j)^c$. Then, we have that, for any $i \in \{1, \ldots, N\}$, $V_i = (G \cap B_i) \cap (\cup_{j=1}^{i-1} B_j)$, and that for any $i_1, i_2 \in \{1, \ldots, K\}, V_{i_1} \cap V_{i_2} = \emptyset$ if $i_1 \neq i_2$. Therefore, we get that $G = \bigcup_{i=1}^K V_i$ and $\Phi_h^{-1}(G) = \bigcup_{i=1}^K \Phi_h^{-1}(V_i)$. In particular, for any $A \in \mathcal{B}(T^*M)$ and any $\zeta \in C_c(T^*M, \mathbb{R})$

$$\int_{G \cap A} \zeta(z)dz = \sum_{i=1}^K \int_{V_i \cap A} \zeta(z)dz,$$

and for any $\tilde{A} \in \mathcal{B}(T^*M)$ and any $\tilde{\zeta} \in C_c(T^*M, \mathbb{R})

$$\int_{\Phi_h^{-1}(G) \cap \tilde{A}} \tilde{\zeta}(z)dz = \sum_{i=1}^K \int_{\Phi_h^{-1}(V_i) \cap \tilde{A}} \tilde{\zeta}(z)dz.$$

Using (58) and (57), we obtain $I' = \sum_{i=1}^K I_i'$, where $I'_i = \int_{V_i \cap \Phi_h^{-1}(G) \cap F_h} g(z, \Phi_h(z))dz$ for any $i \in [K]$. We are now going to show that, for any $i \in [K]$,

$$I'_i = \int_{\Phi_h^{-1}(V_i) \cap G \cap F_h} g(\Phi_h(z), z)dz.$$

Let $i \in [K]$. We proceed by making the following case disjunction:

(a) Either $V_i \cap \Phi_h^{-1}(G) \cap F_h = \emptyset$, and then $I'_i = 0$. We prove by contradiction in this case that $\Phi_h^{-1}(V_i) \cap G \cap F_h = \emptyset$. Assume that there exists $z \in \Phi_h^{-1}(V_i) \cap G \cap F_h$. By definition of $F_h, z \in A_h, \Phi_h(z) \in A_h,$ and we get that $\Phi_h(\Phi_h(z)) = z$ using A3. Hence, we have:

(a) $\Phi_h(z) \in V_i$,

(b) $\Phi_h(\Phi_h(z)) = z \in G$,

(c) $\Phi_h(z) \in A_h$,

(d) $\Phi_h(\Phi_h(z)) = z \in A_h$.

Therefore, we get $\Phi_h(z) \in V_i \cap \Phi_h^{-1}(G) \cap F_h = \emptyset$, which is absurd. Finally, (60) holds since

$$I'_i = 0 = \int_{\Phi_h^{-1}(V_i) \cap G \cap F_h} g(\Phi_h(z), z)dz.$$

(b) Either, there exists some $\tilde{z} \in V_i \cap \Phi_h^{-1}(G)$ such that $\tilde{z} \in F_h$. In particular, $\tilde{z} \in B_1$, and thus $\|\tilde{z} - z_i\|_{z_i} < r(z_i) < 1$. In this case, by combining A3 with Lemma 12(c), we have for any $z' \in T^* M$

$$\|z'\|_z \leq (1 - \|\tilde{z} - z_i\|_{z_i})^{-1} \|z'\|_{z_i} < (1 - r(z_i))^{-1} \|z'\|_{z_i}.$$ 

By considering $z' = z_i - \tilde{z}$, it comes that

$$\|z_i - \tilde{z}\|_z < (1 - r(z_i))^{-1} \|\tilde{z} - z_i\|_{z_i} < (1 - r(z_i))^{-1} r(z_i).$$ 

By combining properties (a) and (b) of $r$ with Lemma 15, we have the following upper bound of $r(z_i)$

$$r(z_i) \leq r(\tilde{z}) + L\|\tilde{z} - z_i\|_2 \leq r(\tilde{z}) + L C_{\pi_i} \|\tilde{z} - z_i\|_{z_i} < r(\tilde{z}) + L C_{\pi_i} r(z_i) < r(\tilde{z}) + 1/4,$$

and thus

$$\|z_i - \tilde{z}\|_z < (1 - r(\tilde{z}) - 1/4)^{-1} (r(\tilde{z}) + 1/4) < 1,$$

using property (c) of $r$. Hence, $z_i \in B_{\|z\|_z}(\tilde{z}, 1)$. Moreover, $\tilde{z} \in F_h \subset A_h$, and then it comes that $h < h_*(z_i)$. Therefore, by combining property (d) of $r$ with A3, we have

(a) $V_i \subset B_i \subset B_{\|z\|_z}(z_i, \lambda r^*(z_i)) \subset \text{dom}_{\Phi_h}$,

(b) the restriction of $\Phi_h$ to $V_i$ is a $C^1$-diffeomorphism such that $\Phi_h \circ \Phi_h = \text{Id}$.

This last result provides proper assumptions on $\Phi_h$ to operate a change of variable in $I_\epsilon'$. We now define $G_{1,h} = \Phi_h(V_i \cap \Phi_h^{-1}(G) \cap F_h)$ and $G_{2,h} = \Phi_h^{-1}(V_i) \cap G \cap F_h$, and prove that $G_{1,h} = G_{2,h}$ in two steps.

(a) We first prove that $G_{1,h} \subset G_{2,h}$. Let $z \in G_{1,h}$. Then, there exists $z' \in V_i \cap \Phi_h^{-1}(G) \cap F_h$ such that $z = \Phi_h(z')$. Since $\Phi_h$ is an involution on $V_i$, we have $\Phi_h(z) = z'$. Since $z' \in V_i \cap A_h$, it comes that $z \in \Phi_h^{-1}(V_i) \cap \Phi_h^{-1}(A_h)$. Moreover, $z' \in \Phi_h^{-1}(G) \cap \Phi_h^{-1}(A_h)$, and thus $z \in G \cap A_h$. Then, we have $z \in G_{2,h}$, which proves this first result.

(b) We now prove that $G_{2,h} \subset G_{1,h}$. Let $z \in G_{2,h}$. In particular, $z \in G$. Then, there exists $j \in [K]$ such that $z \in V_j$. Therefore, $z \in B_j$ and thus $\|z - z_j\|_{z_j} < r(z_j) < 1$. Since $z \in A_h$, we obtain that $h < h_*(z_j)$ with the same computations as those written above. In particular, this proves with A3 that $\Phi_h$ is an involution on $V_j$. Then, $z = \Phi_h(\Phi_h(z))$, with $\Phi_h(z) \in V_i \cap A_h$ and $\Phi_h(z) \in \Phi_h^{-1}(G) \cap \Phi_h^{-1}(A_h)$, since $z \in G \cap A_h$. Therefore, we have $z \in G_{1,h}$, which proves this last result.

Given the fact that $\Phi_h$ is an involution on $V_i$, we operate the change of variable $z \mapsto \Phi_h(z)$ in $I_\epsilon'$ and obtain

$$I_\epsilon' = \int_{\Phi_h(V_i \cap \Phi_h^{-1}(G) \cap F_h)} g(\Phi_h(z), z) \, dz = \int_{\Phi_h^{-1}(V_i) \cap G \cap F_h} g(\Phi_h(z), z) \, dz,$$

which gives (60).

Therefore, combining (58), (59) and (60), we get

$$I' = \sum_{i=1}^K \int_{V_i \cap \Phi_h^{-1}(G) \cap F_h} g(z, \Phi_h(z)) \, dz = \sum_{i=1}^K \int_{\Phi_h^{-1}(V_i) \cap G \cap F_h} g(\Phi_h(z), z) \, dz = J',$$

which concludes the proof.

We are now ready to establish the reversibility up to momentum reversal of $Q_1$, defined in (54), with respect to $\bar{\pi}$.

**Lemma 30.** Assume A1, A2, A3. Then, for any $h > 0$, the Markov kernel $Q_1$ with step-size $h$, defined in (54), is reversible up to momentum reversal with respect to $\bar{\pi}$.

**Proof.** Assume A1, A2, A3. Let $h > 0$. We recall that the kernels $Q_1$ and $Q_2$ are respectively defined in (54) and (55). We define the transition kernel $Q_3 : T^* M \times B(T^* M) \to [0, 1]$ by

$$Q_3(z, dz') = \mathbb{I}_{\bar{E}_h^+(z)} Q_2(z, dz') + \mathbb{I}_{(\bar{E}_h^+)'}(z) \delta_z (dz'),$$

such that $Q_1 = s_# Q_3$. The rest of the proof is divided into two parts. First, we prove that $Q_3$ is reversible with respect to $\bar{\pi}$. Then, we prove that $Q_1$ is reversible up to momentum reversal with respect to $\bar{\pi}$. 

\[\]
(a) Let \( f \in C(\mathbb{T} \times \mathbb{T} \times \mathbb{T}, \mathbb{R}) \) with compact support. We consider a compact set \( K \) with respect to the topology induced by the set \( \{b \| z, r, z \in \mathbb{T} \times \mathbb{T}, r \in (0, 1)\} \) such that \( \text{supp}(f) \subset K \times K \). According to Definition 7, we aim to show that
\[
I = \int_{\mathbb{T} \times \mathbb{T}} f(z, z') \mathbb{Q}_3(z, dz') \mathbb{M}(dz) = \int_{\mathbb{T} \times \mathbb{T}} f(z', z) \mathbb{Q}_3(z, dz') \mathbb{M}(dz) .
\]
We denote by \( I \) the left integral of (62). By combining (55) and (61), we have \( I = I_1 + I_2 + I_3 \) where
\[
I_1 = \int_{\hat{E}_\mathbb{R}} \hat{\pi}(z) a(\mathbb{R}^\Phi(z) | z) f(z, \mathbb{R}^\Phi(z)) dz ,
I_2 = \int_{\hat{E}_\mathbb{R}} \hat{\pi}(z)[1 - a(\mathbb{R}^\Phi(z) | z)] f(z, z) dz ,
I_3 = \int_{\hat{E}_\mathbb{R}} \hat{\pi}(z) f(z, z) dz .
\]
Since \( \text{supp}(f) \subset K \times K \), we have for any \( z \in K^c \), \( f(z, \cdot) = 0 \) and \( f(\cdot, z) = 0 \). Note also that for any \( z \in ((\mathbb{R}^\Phi)^{-1}(K))^c \), \( \mathbb{R}^\Phi(z) \notin K \), and thus \( f(\mathbb{R}^\Phi(z), \cdot) = 0 \) and \( f(\cdot, \mathbb{R}^\Phi(z)) = 0 \). By combining these preliminary results with (6), we get
\[
I_1 = \int_{\hat{E}_\mathbb{R} \cap \mathbb{K} \cap (\mathbb{R}^\Phi)^{-1}(K)} \hat{\pi}(z) a(\mathbb{R}^\Phi(z) | z) f(z, \mathbb{R}^\Phi(z)) dz
dd
(1/Z) \int_{\hat{E}_\mathbb{R} \cap \mathbb{K} \cap (\mathbb{R}^\Phi)^{-1}(K)} \min\{e^{-H(z)}, e^{-H(\mathbb{R}^\Phi(z))}\} f(z, \mathbb{R}^\Phi(z)) dz
I_2 = \int_{\hat{E}_\mathbb{R} \cap \mathbb{K}} \hat{\pi}(z)[1 - a(\mathbb{R}^\Phi(z) | z)] f(z, z) dz ,
I_3 = \int_{\hat{E}_\mathbb{R}} \hat{\pi}(z) f(z, z) dz .
\]
We denote by \( J \) the right integral of (62). By symmetry, we have \( J = J_1 + J_2 + J_3 \) where
\[
J_1 = \int_{\hat{E}_\mathbb{R} \cap \mathbb{K} \cap (\mathbb{R}^\Phi)^{-1}(K)} \hat{\pi}(z) a(\mathbb{R}^\Phi(z) | z) f(\mathbb{R}^\Phi(z), z) dz
(1/Z) \int_{\hat{E}_\mathbb{R} \cap \mathbb{K} \cap (\mathbb{R}^\Phi)^{-1}(K)} \min\{e^{-H(z)}, e^{-H(\mathbb{R}^\Phi(z))}\} f(\mathbb{R}^\Phi(z), z) dz
J_2 = \int_{\hat{E}_\mathbb{R} \cap \mathbb{K}} \hat{\pi}(z)[1 - a(\mathbb{R}^\Phi(z) | z)] f(z, z) dz ,
J_3 = \int_{\hat{E}_\mathbb{R}} \hat{\pi}(z) f(z, z) dz .
\]
We directly have \( I_2 = J_2 \) and \( I_3 = J_3 \). Let us now prove that \( I_1 = J_1 \).
We recall that \( s \circ S_{h/2} \) is a symplectic \( C^1 \)-diffeomorphism (see Section 4.1) and \( \hat{E}_\mathbb{R} = (s \circ S_{h/2})(\mathbb{F}_h) \) where \( \mathbb{F}_h = \mathbb{A}_h \cap \mathbb{Phi}_h^{-1}(\mathbb{A}_h) \), using (53). We define \( \mathbb{K}_h = \mathbb{F}_h \cap (s \circ S_{h/2})(\mathbb{K}) \cap \mathbb{Phi}_h^{-1}((s \circ S_{h/2})(\mathbb{K})) \), such that \( \hat{E}_\mathbb{R} \cap \mathbb{K} \cap (\mathbb{R}^\Phi)^{-1}(K) = (s \circ S_{h/2})(\mathbb{K}_h) \), and we operate the change of variable \( z \mapsto (s \circ S_{h/2})(z) \) in \( I_1 \) and \( J_1 \)
\[
I_1 = (1/Z) \int_{\mathbb{K}_h} \min\{e^{-H((s \circ S_{h/2})(z))}, e^{-H((s \circ S_{h/2} \circ \mathbb{Phi}_h)(z))}\} f((s \circ S_{h/2})(z), (s \circ S_{h/2} \circ \mathbb{Phi}_h)(z)) dz ,
J_1 = (1/Z) \int_{\mathbb{K}_h} \min\{e^{-H((s \circ S_{h/2})(z))}, e^{-H((s \circ S_{h/2} \circ \mathbb{Phi}_h)(z))}\} f((s \circ S_{h/2} \circ \mathbb{Phi}_h)(z), (s \circ S_{h/2})(z)) dz .
\]
We now define the map \( g : \mathbb{T} \times \mathbb{T} \times \mathbb{T} \to \mathbb{R} \) and the set \( G \subset \mathbb{T} \times \mathbb{T} \) by
\[
g(z, z') = \min\{e^{-H((s \circ S_{h/2})(z))}, e^{-H((s \circ S_{h/2} \circ \mathbb{Phi}_h)(z))}\} f((s \circ S_{h/2})(z), (s \circ S_{h/2})(z')) ,
G = (s \circ S_{h/2})(\mathbb{K}) .
\]
Note that \( G \) is a compact set of \( \mathbb{T} \times \mathbb{T} \times \mathbb{T} \) by continuity of \( s \circ S_{h/2} \) and \( g \) is a continuous function by continuity of \( H \) and \( s \circ S_{h/2} \). Then, we obtain \( I_1 = J_1 \), by applying Lemma 29 with \( g \) and \( G \). Finally, we obtain \( I = J \) and thus prove (62) for any continuous function \( f \) with compact support.

(b) Let \( f : \mathbb{T} \times \mathbb{T} \times \mathbb{T} \to \mathbb{R} \) be a continuous function with compact support. We have
\[
I = \int_{\mathbb{T} \times \mathbb{T}} f(z, z') \mathbb{Q}_1(z, dz') \mathbb{M}(dz) = \int_{\mathbb{T} \times \mathbb{T}} f(z, z') \mathbb{Q}_3(z, dz') \mathbb{M}(dz)
\]
\[
= \int_{\mathbb{T} \times \mathbb{T}} f(z, s(z)) \mathbb{Q}_3(z, dz') \mathbb{M}(dz) \quad \text{(momentum reversal on } z')
\]
\[
= \int_{\mathbb{T} \times \mathbb{T}} f(z', s(z)) \mathbb{Q}_3(z, dz') \mathbb{M}(dz) \quad \text{(using (62))}
\]
\[
= \int_{\mathbb{T} \times \mathbb{T}} f(s(z'), s(z)) \mathbb{Q}_3(z, dz') \mathbb{M}(dz) \quad \text{(momentum reversal on } z')
\]
which concludes the proof.
We are now ready to prove Theorem 6, which states that $Q$ is reversible up to momentum reversal with respect to $\bar{\pi}$.

**Proof of Theorem 6.** Assume A1, A2, A3. This proof is very similar to the proof of Theorem 4 (see Appendix D.2). Let $f : T^{*}M \times T^{*}M \to \mathbb{R}$ be a continuous function with compact support. We have

$$
\int_{T^{*}M \times T^{*}M} f(z, z') Q(z, dz') \bar{\pi}(dz) \\
= \int_{T^{*}M \times T^{*}M \times T^{*}M \times T^{*}M} f(z, z') Q_0(z, dz_1) Q_1(z_1, dz_2) Q_0(z_2, dz') \bar{\pi}(dz) \\
(\text{see (56)}) \\
= \int_{T^{*}M \times T^{*}M \times T^{*}M} f(s(z_1), z') Q_0(z, dz_1) Q_1(s(z), dz_2) Q_0(z_2, dz') \bar{\pi}(dz) \\
(\text{Lemma 17}) \\
= \int_{T^{*}M \times T^{*}M \times T^{*}M} f(s(z_1), z') Q_0(z_2, dz_1) Q_1(z, dz_2) Q_0(s(z), dz') \bar{\pi}(dz) \\
(\text{momentum reversal on } z) \\
= \int_{T^{*}M \times T^{*}M \times T^{*}M} f(s(z_1), z') Q_0(z_2, dz_1) Q_1(z, dz_2) Q_0(z, dz') \bar{\pi}(dz) \\
(\text{Lemma 30}) \\
= \int_{T^{*}M \times T^{*}M \times T^{*}M} f(s(z_1), s(z)) Q_0(z_2, dz_1) Q_1(z', dz_2) Q_0(z, dz') \bar{\pi}(dz) \\
(\text{momentum reversal on } z) \\
= \int_{T^{*}M \times T^{*}M} f(s(z'), s(z)) Q(z, dz') \bar{\pi}(dz) .
$$

Moreover, $s_* \bar{\pi} = \bar{\pi}$. Hence, by combining Definition 7 and Lemma 8, we obtain the result of Theorem 6.

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**I Experimental details and additional results**

In this section, we first give more details about our experimental setup. Then, we detail an ablation study regarding the randomness of the step-size. Third, we give more details about the stability of our algorithm in the case of the Birkhoff polytope. In particular, we highlight that, as a by-product, our reversibility check seems to prevent numerical instability.

**Experimental setup.** We used a cluster with three nodes (12 cores, 2.9 GHz, 192Go, CentOS 7), (16 cores, 2.4 GHz, 256Go, CentOS 7), (8 cores, 3.3GHz, 128Go, CentOS 7) to perform our hyperparameter sweeps. At each iteration, we perform one step of numerical integration. It is not clear how to extend our theoretical framework to the case where more than one integration step is performed. In particular, it is unclear if the reversibility is preserved in that framework and if not, what are the required modifications to recover the reversibility. Early experiments with a reversibility check performed at the end of 10 integration steps (instead of considering only 1 integration step) were associated with slow mixing Markov chains with a sticking behaviour at the boundaries. In our code we implement both the Störmer-Verlet and the implicit midpoint methods. The implicit midpoint method replaces (4) with

$$
p^{(1)} = p^{(0)} - h \partial_p H_2((x^{(0)} + x^{(1)})/2, (p^{(0)} + p^{(1)})/2) , \\
x^{(1)} = x^{(0)} + h \partial_x H_2((x^{(0)} + x^{(1)})/2, (p^{(0)} + p^{(1)})/2) .
$$

Note that in theory we could not prove the existence of diffeomorphisms, see Section 5.1, with our approach using the midpoint method. The main difficulty resides in the fact that we cannot easily express $p^{(0)}$ as a function of $x^{(1)}$ and $x^{(0)}$, which is explicit in the case of the Störmer-Verlet. In practice, we did not notice any noticeable difference between the Störmer-Verlet integrator and the midpoint integrator and use only the Störmer-Verlet integrator. We refer to Appendix E for more details on the differences between these integrators. On a few early runs we did not notice a noticeable impact of the parameter $\beta$ and decided to keep $\beta = 1$ for simplicity. In order to numerically approximate the Störmer-Verlet integrator, we use $K = 10$ fixed point iterations. We also implemented a second-order (Newton method) to numerically approximate the Störmer-Verlet integrator but found that this approximation scheme gave similar results and was slower to run at each step (due to the need of computing additional matrix products). We therefore approximate the Störmer-Verlet integrator using only the fixed point iterations. In order to assess that the obtained transformation are volume preserving we compute $|1 - \det(D\Phi_h([x', p']))|$ at each iteration of the dynamics. We compute these differential operators using the jax.jacfwd command which performs (forward-mode) automatic differentiation by unrolling the numerical integrator. In Figure 7 we plot some of these errors in logarithmic scale for different values of $K$. We note that we get errors of order $10^{-6}$ as soon as $K = 10$ iterations. Choosing more iterations $K = 20$ does not significantly reduce the error and therefore we keep the value $K = 10$. 

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Influence of the random step-size. We incorporate a random step-size in the algorithm by sampling uniformly on $(0, h)$. Empirically, we notice that incorporating this random step-size was beneficial to the stability of the algorithm. In Table 3 we present a study where we vary $\eta$ (the tolerance threshold) for $h = 0.8$ and $600k$. We consider 2 frameworks: random step-size (Rand) or fixed step-size (NoRand). If $\eta = + \infty$ then no reversibility check is performed.

Table 3: Results for $h = 0.3$ after 800k iterations of n-BHMC (average over 3 runs).

| Setting         | square     | cosine | FSR     | BSR     |
|-----------------|------------|--------|---------|---------|
| (NoRand) $\eta = + \infty$ | $0.276_{\pm 0.006}$ | $0.695_{\pm 0.006}$ | $0.81$ | $1.00$ |
| (NoRand) $\eta = 10^{-2}$     | $0.303_{\pm 0.001}$ | $0.668_{\pm 0.001}$ | $0.82$ | $0.55$ |
| (NoRand) $\eta = 10^{-3}$     | $0.288_{\pm 0.001}$ | $0.684_{\pm 0.001}$ | $0.82$ | $0.45$ |
| (NoRand) $\eta = 10^{-4}$     | $0.284_{\pm 0.002}$ | $0.687_{\pm 0.002}$ | $0.82$ | $0.35$ |
| (Rand) $\eta = + \infty$      | $0.311_{\pm 0.001}$ | $0.659_{\pm 0.001}$ | $0.93$ | $1.00$ |
| (Rand) $\eta = 10^{-2}$       | $0.333_{\pm 0.004}$ | $0.637_{\pm 0.004}$ | $0.92$ | $0.85$ |
| (Rand) $\eta = 10^{-3}$       | $0.322_{\pm 0.004}$ | $0.647_{\pm 0.004}$ | $0.92$ | $0.78$ |
| (Rand) $\eta = 10^{-4}$       | $0.320_{\pm 0.005}$ | $0.653_{\pm 0.005}$ | $0.92$ | $0.70$ |

Similarly as in Section 7, we denote in blue the results obtained using the reversibility check and in bold the results such that the true values ($1/3$ in the case of square and $2/\pi$ in the case of cosine) are in the confidence interval. At first, the results of Table 3 might seem counterintuitive since a lower tolerance $\eta$ is supposed to produced less bias. However, we observe that by reducing $\eta$ we also harm the mixing time of the Markov chain and therefore it takes a long time to reach convergence. Note that in all settings choosing a random step-size improved reduced the bias. Hence, with a finite computational budget, one must choose a value of $\eta$ such that (a) the bias is reduced (b) the tolerance threshold does not harm the convergence of the chain too much. In practice we have observed that the choice of a good tolerance parameter is dependent on the computational budget, the dimension of the problem, the type of constraints and the step-size $h$ used in HMC. We leave for future work a more thorough study aimed at giving principled guidelines for the choice of $\eta$.

Stability in the Birkhoff polytope. We elaborate on what we mean by stability in the case of the Birkhoff polytope. Indeed, we observe that in dimension 16 ($5 \times 5$ doubly stochastic matrices) using a step-size $h = 0.3$, 6 out of 6 runs without reversibility check are hitting NaN at some point when computing the barrier, whereas with the reversibility check only 1 run out of 6 was hitting NaN at some point when computing the barrier. Without reversibility check NaN are obtained after only $5k$ iterations in average. The Markov chains are run for a total of $500k$ iterations. The other parameters of the samplers are fixed as follows. We consider $K = 10$ iterations in the fixed point algorithm to solve the Störmer-Verlet integrator. The tolerance is fixed to $\eta = 10^{-2}$ and $\beta = 1$. We emphasize that we do not observe such explosive behavior if we set $h = 0.1$. Note that under the same setting, a similar behavior is observed in the case of the simplex after $50k$ iterations.

In Figure 8, we illustrate the behavior of the algorithm by plotting the running average of the sampled matrices which should converged to the mean of the uniform distribution on the Birkhoff polytope, i.e. the matrix filled with $1/n$ for a $n \times n$ matrix.

Examples of the simplex and with a potential. In this last section, we illustrate our algorithm to sample from the uniform on the simplex and from a distribution on the hypercube which is not uniform. We plot samples and the autocorrelation function in Figure 9 for a target $\pi$ such that for any $x \in \mathbb{R}^d$ we have

$$(d\pi/d\text{Leb})(x) = \exp[-\|x - \mu\|^2/(2\sigma^2)] \mathbb{1}_{[-1,1]}(x) / \int_{[-1,1]} \exp[-\|\tilde{x} - \mu\|^2/(2\sigma^2)] d\tilde{x}.$$
In our experiment, we take $\mu = (1, 1)$ and $\sigma = 0.5$. We fix $h = 0.3$ and $\eta = 10^{-2}$. We use the Störmer-Verlet integrator with $K = 10$ fixed point iterations.

Finally, we conclude with samples from another polytope with hard constraints. We consider the simplex given by $\Delta_d = \left\{ x \in (0, +\infty)^d : \sum_{i=1}^d x_i = 1 \right\}$. We use $K = 10$ iterations in the fixed point algorithm to solve the Störmer-Verlet integrator. The tolerance is fixed to $\eta = 10^{-2}$ and $\beta = 1$. As emphasized in the previous paragraph, without reversibility check we observe NaN values after $50k$ iterations. This is not the case if we include a reversibility check. We assess the efficiency of the algorithm in Figure 10.