Abstract

Markov chain Monte Carlo (MCMC) algorithms offer various strategies for sampling; the Hamiltonian Monte Carlo (HMC) family of samplers are MCMC algorithms which often exhibit improved mixing properties. The recently introduced magnetic HMC, a generalization of HMC motivated by the physics of particles influenced by magnetic field forces, has been demonstrated to improve the performance of HMC. In many applications, one wishes to sample from a distribution restricted to a constrained set, often manifested as an embedded manifold (for example, the surface of a sphere). We introduce magnetic manifold HMC, an HMC algorithm on embedded manifolds motivated by the physics of particles constrained to a manifold and moving under magnetic field forces. We discuss the theoretical properties of magnetic Hamiltonian dynamics on manifolds, and introduce a reversible and symplectic integrator for the HMC updates. We demonstrate that magnetic manifold HMC produces favorable sampling behaviors relative to the canonical variant of manifold-constrained HMC.

1 INTRODUCTION

Markov chain Monte Carlo (MCMC) is an important class of inference algorithm which has revolutionized inference in Bayesian statistical models. Originally developed by physicists, MCMC owes much to physical inspiration, including two popular techniques for Bayesian inference: the Metropolis-adjusted Langevin diffusion [Roberts and Stramer, 2002] and Hamiltonian Monte Carlo (HMC) [Duane et al., 1987]. These methods may be straightforwardly applied to sample from differentiable densities on Euclidean spaces. For the history of MCMC, see [Diaconis, 2009; Robert and Casella, 2011].

Our purpose is to expand on the HMC literature for non-Euclidean spaces by continuing to draw on physics for inspiration. Examples of manifolds of interest that may be equipped with densities include the sphere, tori, the special orthogonal group (n-dimensional rotation matrices), and the Stiefel manifold (n x m matrices with orthogonal columns). Important contributions in these directions include Byrne and Giro [2013] and Brubaker et al. [2012] which develop symmetric and volume-preserving integrators based on closed-form geodesics and the generalized leapfrog algorithm, respectively.

However both of these methods, and virtually all HMC procedures besides, are based on canonical formalism of Hamiltonian dynamics from symplectic geometry. A notable exception is [Tripuraneni et al., 2017] which develops “magnetic HMC” for Euclidean spaces; magnetic HMC considers Markov chain transitions for Hamiltonian dynamics with magnetic field effects. In this work, we examine the foundations of Hamiltonian dynamics from the perspective of symplectic geometry on embedded manifolds. We propose a variant of Hamiltonian dynamics which does not conform to the canonical formalism. Instead, motion generated by these dynamics corresponds to the motion of a particle undergoing potential, magnetic field, and manifold constraint forces simultaneously. Using these dynamics as a transition mechanism, we formulate a method called magnetic manifold HMC. Although the underlying dynamics have a physical interpretation, an understanding of the physics is not critical for understanding magnetic manifold HMC as a sampler. In our experimental evaluation, we show that magnetic manifold HMC produces better sampling behaviors in manifold-constrained inference tasks. Magnetic manifold HMC has a degree of freedom in the choice of a magnetic structure. Our experiments suggest that different choices of magnetic structures tend to recover different modes; therefore, multiple runs with differ-
ent magnetic structures can be used to improve not only the local sampling properties of HMC, but also the exploration of different modalities of the posterior.

The outline of this paper is as follows. In section 2 we examine key concepts such as symplecticsness of a map, numerical integration, and Hamiltonian mechanics on embedded manifolds. In section 3 we review the theory of Hamiltonian dynamics for use in a MCMC procedure for random variables that are constrained to a manifold. Section 4 introduces the magnetic manifold. Section 5 introduces the magnetic manifold HMC algorithm on inference tasks.

The exploration of different modalities of the posterior.

2 PRELIMINARIES

This section contains preliminary material to understand the majority of our paper. Topics include a construction of Hamiltonian mechanics, techniques and notions from embedded manifolds, and methods of numerical integration. The proofs in section 5 require methods from differential geometry; preliminary material for these are in appendix A. Throughout, we denote the $m \times m$ identity matrix by $\text{Id}_m$ and the $m \times m$ zero matrix by $0_m$. The set of skew-symmetric $m \times m$ matrices is denoted $\text{Skew}(m)$.

2.1 Embedded Manifolds

In many cases, a manifold $M$ can be embedded in a Euclidean space $\mathbb{R}^m$ as the preimage of a constraint function $g : \mathbb{R}^m \to \mathbb{R}^k$ on the level set where $g$ takes the value zero: $M \overset{\text{def.}}{=} \{ q \in \mathbb{R}^m : g(q) = 0 \}$. We denote the Jacobian of $g$ at the point $q \in M$ by $G(q)$. For any point $q \in M$, $G(q)$ is a $k \times m$ matrix. We assume that $G(q)$ is full-rank for any $q \in M$. Many manifolds of interest may be written in this way such as the sphere, the special orthogonal group, the Stiefel manifold, and tori, among others. We define several important concepts related to embedded manifolds.

**Definition 1** (Tangent Space). Let $q \in M$. The tangent space at $q$, denoted $T_qM$, is the set of vectors satisfying,

$$T_qM \overset{\text{def.}}{=} \{ \xi \in \mathbb{R}^m : G(q)\xi = 0 \}. \quad (1)$$

where $G$ is the Jacobian of the constraint function $g$.

**Definition 2** (Cotangent Space). The cotangent space at $q$, denoted $T_q^*M$, is the set of vectors,

$$T_q^*M \overset{\text{def.}}{=} \{ p \in \mathbb{R}^m : G(q)\nabla_p H(q,p) = 0 \}, \quad (2)$$

where $H : \mathbb{R}^m \times \mathbb{R}^m \to \mathbb{R}$ is a smooth function.

The dependence of the cotangent space on the function $H$ is suppressed by convention. The tangent space is a vector space. When $G(q)\nabla_p H(q,p)$ is a linear function of $p$, the cotangent space is also a vector space.

**Definition 3** (Cotangent Bundle). The set of vectors,

$$T^*M \overset{\text{def.}}{=} \{ (q,p) \in \mathbb{R}^m \times \mathbb{R}^m : q \in M \text{ and } p \in T_q^*M \} \quad (3)$$

is called the cotangent bundle.

**Definition 4.** The embedding of $T^*M$ in $\mathbb{R}^{2m}$ is defined to be the set of vectors

$$\{ (q,p) \in \mathbb{R}^{2m} : g(q) = 0 \text{ and } G(q)\nabla_p H(q,p) = 0 \} \quad (4)$$

**Definition 5** (Linear Maps between Tangent Spaces). Let $M$ be a manifold. Let $\Phi : M \to M$ be a smooth function. Then $T_q\Phi : T_qM \to T_{\Phi(q)}M$ is the linear mapping obtained by differentiating $\Phi$ at $q$. We use the notation $(T_q\Phi)u$ to represent the linear map applied to $u$ yielding a vector in $T_{\Phi(q)}M$. When $M$ is embedded in Euclidean space, $(T_q\Phi)u = \nabla\Phi(q)^\top u.$

**Definition 6** (Pullback). Given a map $\Omega : T_qM \times T_qM \to \mathbb{R}$, its pullback by a smooth function $\Phi : M \to M$ is the map $\Phi^*\Omega$ defined by $(\Phi^*\Omega)(u,v) \overset{\text{def.}}{=} \Omega((T_q\Phi)u,(T_q\Phi)v)$ where $u,v \in T_qM$. $2.2$ Hamiltonian Mechanics

Hamiltonian mechanics are classically formulated as differential equations on the cotangent bundle of a smooth manifold $M$. Formally, given a manifold $M$, Hamiltonian mechanics give the time evolution of a point $(q,p) \in T^*M$, often called phase-space in physics wherein $p$ is called the momentum. Recall that $T^*M$ is an embedded manifold from definition 4.

Our construction of Hamiltonian mechanics requires the specification of an object called the symplectic structure. One formulation of the symplectic structure uses a matrix associated with it. Let $\mathbb{J} \in \text{Skew}(2m)$ be an invertible, skew-symmetric matrix. Let $u,v \in T_{(q,p)}T^*M$ (i.e., two vectors, each in the tangent space to the cotangent space $T^*M$, which is a manifold) with $u = (u_1, \ldots, u_{2m})$ and $v = (v_1, \ldots, v_{2m})$.

**Definition 7** (Symplectic Structure). The skew-symmetric, bilinear map $\Omega : T_{(q,p)}T^*M \times T_{(q,p)}T^*M \to \mathbb{R}$ defined by $\Omega(u,v) = u^\top \mathbb{J} v$ is called a symplectic structure on $T^*M$ with matrix $\mathbb{J}$.

**Definition 8** (Symplectic Transformation). A map $\Phi : T^*M \to T^*M$ is symplectic if $\Phi^*\Omega = \Omega$, where $\Phi^*\Omega$ is the pullback (definition 6) of $\Omega$ by $\Phi$. Magnetic Manifold Hamiltonian Monte Carlo
Given a symplectic structure on $T^*M$, we provide a definition of Hamilton’s equations of motion.

**Definition 9 (Hamiltonian Vector Field).** Let $\Omega$ be a symplectic structure on $T^*M$ and let $H : \mathbb{R}^m \times \mathbb{R}^m \to \mathbb{R}$ be a smooth function; $H$ is called the Hamiltonian. Let $(q, p) \in T^*M$ and let $T_{(q,p)}T^*M$ be the tangent space of $T^*M$ at $(q, p)$. The unique Hamiltonian vector field $X_H : T^*M \to TT^*M$ satisfies $\Omega(X_H(q, p), \delta) = \langle T_{(q,p)}H \rangle \delta$ for all $\delta \in T_{(q,p)}T^*M$.

**Definition 10 (Hamiltonian Vector Field Flows).** The flow of a Hamiltonian vector field $X_H : T^*M \to TT^*M$ to time $t$ is the map $\Phi(\cdot; t) : T^*M \to T^*M$ satisfying $\frac{d}{dt} \Phi(q, p; t) = X_H(\Phi(q, p; t))$ and $\Phi(q, p; 0) = (q, p)$ for $(q, p) \in T^*M$.

**Definition 11 (Hamilton’s Equations of Motion).** Suppose $(q_t, p_t) = \Phi(q, p; t)$. Since $\frac{d}{dt} \Phi(q, p; t) = X_H(\Phi(q, p; t))$, we have derived the equations of motion $(q_t, p_t) = X_H((q_t, p_t))$.

The choice of symplectic form $\Omega$ affords a degree of freedom to Hamiltonian mechanics. The following example gives the form of $\Omega$ which recovers the canonical Hamiltonian equations of motion in Euclidean space.

**Example 1.** When $M \cong \mathbb{R}^m$, we have that $T^*M \cong \mathbb{R}^{2m}$. The canonical symplectic structure $\Omega_{\text{can}}$ is a bilinear map from $\mathbb{R}^{2m} \times \mathbb{R}^{2m}$ to $\mathbb{R}$ with matrix

$$J_{\text{can}} = \begin{pmatrix} 0_m & I_{2m} \\ -I_{2m} & 0_m \end{pmatrix} \in \text{Skew}(2m).$$

such that $\Omega(\delta_1, \delta_2) = \delta_1^T J_{\text{can}} \delta_2$ for $\delta_1, \delta_2 \in \mathbb{R}^{2m}$. Definition 9 produces the familiar equations of motion $\dot{q}_t = \nabla_p H(q_t, p_t)$ and $\dot{p}_t = -\nabla_q H(q_t, p_t)$. Hence the constraint $G(q) \nabla_p H(q, p) = 0$ in definition 4 means the velocity is constrained to the tangent space.

### 2.3 Numerical Integration

For most Hamiltonian vector fields, even those on Euclidean space, there do not exist closed-forms for the flows. Therefore, it is necessary to design numerical integrators for Hamiltonian systems.

**Definition 12 (Numerical Integrator).** A numerical integrator of a Hamiltonian system with step-size $\epsilon \in \mathbb{R}$ and number of integration steps $N \in \mathbb{N}$ is a map $\Phi(\cdot; \epsilon; N) : T^*M \to T^*M$ approximating $\Phi(\cdot; \epsilon; N)$.

While a good approximation is desirable in HMC for high acceptance probabilities, the quality of approximation is of no consequence for the correctness of the sampler. However, it is essential for our formulation of HMC that numerical integrators are symmetric and symplectic, defined as follows.

**Definition 13 (Symmetric Map).** A map $\Phi : T^*M \to T^*M$ is symmetric if $\Phi(\Phi(z; -\epsilon); \epsilon) = z$ for all $z \in T^*M$.

**Definition 14 (Symmetric Integrator).** A numerical integrator $\Phi$ is symmetric if, for fixed $N$, $\Phi(\cdot; \epsilon, N)$ is a symmetric map for all $\epsilon$.

**Definition 15 (Symplectic Integrator).** A numerical integrator is symplectic if, for fixed $\epsilon$ and $N$, the map $\Phi(\cdot; \epsilon, N)$ is symplectic (definition 8).

Symplectic integrators preserve volume in $T^*M$ in the following sense; for details see appendix K.

**Definition 16 (Volume Preserving).** A numerical integrator is volume preserving if for any region $Z \subset T^*M$ with volume $\text{Vol}(Z)$ the set $Z' \text{ def} = \{ \Phi(q, p; \epsilon, N) : (q, p) \in Z \}$ satisfies $\text{Vol}(Z) = \text{Vol}(Z')$ for any choice of $\epsilon$ and $N$.

Flows of Hamiltonian vector fields are symmetric and symplectic: this fact, in combination with the technique of Strang splitting (MacNamara and Strang, 2011), forms the basis of many symplectic integrators.

### 3 RELATED WORK

Our methodology is based on the HMC algorithm which is originally due to Duane et al. (1987). Two avenues of research are of immediate relevance to the present research. The first of these is research into non-canonical HMC, which explores non-canonical symplectic structures and their usefulness for inference. Magnetic HMC (Tripuraneni et al., 2017) is a special case of non-canonical HMC using a symplectic structure corresponding to motion of a particle in a magnetic field. Non-canonical HMC was further explored in [Brofos and Lederman, 2020], which proposed an explicit integration strategy for a broad class of non-canonical, constant symplectic structures. The second avenue of research most related to our work is (canonical) HMC on manifolds. In Girolami and Calderhead (2011), the authors consider inference on Riemannian manifolds with global coordinates. Brubaker et al. (2012) expands on this work by proposing an integrator suitable for embedded manifolds of Euclidean space via the method of Lagrange multipliers. An alternative approach was pursued in Byrne and Girolami (2013) wherein the Lagrange multipliers are eliminated by formulating an integrator using closed-form geodesics on embedded manifolds.

### 4 HMC ON MANIFOLDS

Let $M$ be a manifold embedded in Euclidean space. A probability density on $M$ is a map $\pi : M \to \mathbb{R}$ satisfying $\pi(q) \geq 0$ for all $q \in M$ and $\int_M \pi(q) \, dq = 1$. We consider the case $\pi(q) \propto \exp(-U(q))$ where $U : \mathbb{R}^m \to \mathbb{R}$ is a smooth function called the potential energy. We consider Hamiltonians that may be
expressed as the sum of the potential energy and another function \(K: \mathbb{R}^m \to \mathbb{R}\) called the kinetic energy: 
\[
H(q, p) = U(q) + K(p).
\]
We restrict our attention to the case of a quadratic potential energy 
\[
K(p) = \frac{1}{2}p^T p.
\]
The Hamiltonians we consider are of the form
\[
H(q, p) = U(q) + \frac{1}{2}p^T p. \tag{6}
\]
Consider a joint distribution on \(T^*M\) defined by 
\[
\pi(q, p) \propto \exp(-H(q, p)) = \exp(-U(q)) \cdot \exp(-p^T p/2).
\]
We recognize the marginal distribution in \(p\) (marginalizing out \(q\)) as a standard normal distribution subject to the constraint that 
\[
p \in T_q^*M. \tag{7}
\]

**Definition 17** (Transition Operator). The transition operator is a (possibly stochastic) map \(Q: T^*M \to T^*M\). A Markov chain consists of repeated application of the transition operator.

**Definition 18** (Transition Density). The transition density \(\Pi_Q((q', p')|(q, p)) \in \mathbb{R}_+\) is the probability density that \(Q(q, p)\) equals \((q', p')\) given that the chain is currently in state \((q, p)\) in \(T^*M\).

**Definition 19** (Stationary Distribution). A distribution \(\pi(q, p)\) is the stationary distribution of a Markov chain with transition density \(\Pi_Q\) if
\[
\int_{T^*M} \pi(q, p) \cdot \Pi_Q((q', p')|(q, p)) dq dp = \pi(q', p'). \tag{8}
\]

**Definition 20** (Detailed Balance). The transition operator \(Q\) satisfies detailed balance with respect to \(\pi(q, p)\) if
\[
\pi(q, p) \cdot \Pi_Q((q', p')|(q, p)) = \pi(q', p') \cdot \Pi_Q((q, p)|(q', p')). \tag{9}
\]

The detailed balance condition says that, for the stationary distribution, the probability of being in state \((q, p)\) and transitioning to the state \((q', p')\) is equal to the probability of being in state \((q', p')\) and transitioning to the state \((q, p)\). If a Markov chain satisfies detailed balance with respect to \(\pi(q, p)\), \(\pi(q, p)\) is the stationary distribution of the chain, which is readily verified by substituting eq. (8) into eq. (7). For a discussion of conditions leading to the uniqueness of the stationary distribution, see Robert and Casella (2005).

### 4.1 Detailed Balance in HMC

Symmetry and symplecticness are important to detailed balance in HMC. The following is reformulation of Theorem 1 from Brubaker et al. (2012).

**Theorem 1.** Let \(M = \{q \in \mathbb{R}^m : g(q) = 0\}\) be a connected manifold such that \(G(q)\) has full-rank. Let \(T^*M\) be an embedded sub-manifold of \(\mathbb{R}^{2m}\) as in 

\[\text{Algorithm 1} \text{ The transition operator for manifold-constrained Hamiltonian Monte Carlo Markov chain.}\]

1. **Parameters:** Hamiltonian \(H(q, p) = U(q) + \frac{1}{2}p^T p\). Manifold \(M = \{q \in \mathbb{R}^m : g(q) = 0\}\) embedded in \(\mathbb{R}^m\). Symmetric and symplectic numerical integrator \(\Phi\).
2. **Input:** Initial position \(q \in M\) and momentum \(p \in T_q^*M\). Number of integration steps \(N \in \mathbb{N}\).
3. **Sample** \(\epsilon \sim \text{DiscreteUniform}(-\epsilon^*, +\epsilon^*)\).
4. **Compute** \((q', p') = \Phi(q, p; \epsilon, N)\).
5. **Sample** \(U \sim \text{Uniform}(0, 1)\).
6. **if** \(U < \min\{1, \exp(H(q, p) - H(q', p'))\} \text{ then} \)
7. **Return:** \((q', p')\).
8. **else**
9. **Return:** \((q, p)\).
10. **end if**

A proof is given in appendix [J]. We give the complete procedure for manifold-constrained HMC in algorithm [G]. To sample from \(\pi(q) \propto \exp(-U(q))\), it suffices to project samples from \(\pi(q, p)\) to their \(q\)-components. For details on HMC see Bishop (2006).

### 4.2 Sampling in the Cotangent Space

Theorem [B] requires sampling \(p \mid q \sim \text{Normal}(0, \text{Id}_m \mid G(q)p = 0)\). Let \(H: T^*M \to \mathbb{R}\) be a smooth Hamiltonian of the form in eq. (6). Let \(\Phi\) be a symmetric (definition [I]) and symplectic (definition [J]) integrator. The transition operator \(Q: T^*M \to T^*M\) constructed in algorithm [G]. The Markov chain with transition operator \(Q\) is stationary for the distribution \(\pi(q, p) \propto e^{-H(q, p)}\).

For all of the manifolds we consider, there exists a closed-form for the orthogonal projection to the cotangent space. Formulas for orthogonal projections may be found in Boumal (2020).

### 5 MAGNETIC MANIFOLD HMC

This section formulates magnetic Hamiltonian mechanics on an embedded manifold. We prove the dynamics are symmetric, symplectic and conserve energy. We propose a numerical integrator that is symmetric and symplectic, the two essential properties of integrators for HMC. As a consequence, we use this integrator in algorithm [G] to construct a Markov chain satisfying detailed balance with respect to the density \(\pi(q, p) \propto \exp(-H(q, p))\) on \(T^*M\). We define the symplectic structure corresponding to magnetic motion.
Definition 21. The magnetic symplectic structure, denoted \( \Omega_{\text{mag}} \), is the symplectic structure with matrix
\[
\mathbb{J}_{\text{mag}} = \begin{pmatrix}
L & \text{Id}_m \\
-L & 0_m
\end{pmatrix}
\]
where \( L \in \text{Skew}(m) \).

According to Dirac’s theory of constraints (Dirac, 1964), it suffices to embed a manifold-constrained Hamiltonian system in a Euclidean space. Consider the motion on \( T^*M \) determined by,
\[
\begin{align*}
\dot{q}_t &= \nabla_p H(q_t, p_t) \\
\dot{p}_t &= -\nabla_q H(q_t, p_t) - L \nabla_p H(q_t, p_t) - G(q_t)\top \lambda_t \\
g(q_t) &= 0
\end{align*}
\]
where \( g : \mathbb{R}^m \to \mathbb{R}^k \) is a constraint function, \( G : \mathbb{R}^m \to \mathbb{R}^{k \times m} \) is the Jacobian of the constraint, and \( \lambda \in \mathbb{R}^k \) is a vector of Lagrange multipliers. The Lagrange multipliers \( \lambda = (\lambda(q_t, p_t)) \) are uniquely defined by the condition \( g(q_t) = 0 \) along solutions of eqs. (10), (11) and (12); see appendix L. These equations of motion correspond to the magnetic vector field flows (definition 22) to time \( \epsilon \) of \( H_1 \) and \( H_2 \) by \( \Phi_1^\epsilon \) and \( \Phi_2^\epsilon \), respectively. For completeness, we restate in appendix G the closed-form expressions for \( \Phi_1^\epsilon \) and \( \Phi_2^\epsilon \), originally introduced in Tripuraneni et al. (2017); see eqs. (134) to (137), specifically. The single-step subroutine in algorithm 2 computes the symmetric composition of Hamiltonian flows \( \Phi_1 \circ \Phi_2 : \mathbb{R}^{2m} \to \mathbb{R}^{2m} \); we note that this composition is defined on \( \mathbb{R}^{2m} \) and not specific to the manifold. We require the following lemma.

Lemma 1 (Symmetry and Symplecticness of Algorithm 2). The single-step integrator for magnetic dynamics in Euclidean space in algorithm 2 is symmetric and symplectic.

A proof is given in appendix G. We propose a manifold-constrained integrator as the following series of updates. At iteration \( n \), let \( (q_n, p_n) \in T^*M \). Compute:
\[
\begin{align*}
\bar{p}_{n+1/2} &= p_n - \frac{\epsilon}{2} G(q_n)\top \mu \\
(q_{n+1}, \bar{p}_{n+1}) &= \Phi_1^\epsilon \circ \Phi_2^\epsilon \circ \Phi_1^\epsilon(q_n, \bar{p}_{n+1/2}) \\
0 &= g(q_{n+1}) \\
p_{n+1} &= \bar{p}_{n+1} - \frac{\epsilon}{2} G(q_{n+1})\top \mu' \\
0 &= G(q_{n+1})\top p_{n+1}.
\end{align*}
\]
Algorithm 2 The procedure for a single step of integrating Euclidean magnetic Hamiltonian trajectories. Closed-forms for $\Phi_1^\prime$ and $\Phi_2^\prime$ may be found in appendix C. This algorithm, and the closed-form flows $\Phi_1^\prime$ and $\Phi_2^\prime$, were derived in [17].

1: Parameters: Hamiltonian $H(q,p) = U(q) + \frac{1}{2}p^\top p$. 
2: Input: Initial position and momentum variables $q_0 \in \mathbb{R}^m$ and $p_0 \in \mathbb{R}^m$. Integration step-size $\epsilon > 0$. 
3: Compute $(q_0, p_0)/2 = \Phi_1^\prime(q_0, p_0)$ where $\Phi_1^\prime$ is defined in eq. (13).
4: Compute $(q_1, p_1)/2 = \Phi_2^\prime(q_0, p_1/2; L)$ where $\Phi_2^\prime$ is defined in eqs. (135) to (137).
5: Compute $(q_1, p_1) = \Phi_1^\prime(q_1, p_1/2)$.
6: Return: $(q_1, p_1)$.

Algorithm 3 The procedure for integrating manifold-constrained magnetic Hamiltonian trajectories. This is a symmetric and symplectic integrator. At each iteration, the pair $(q_{n+1}, p_{n+1}) \in T^* M$.

1: Parameters: Hamiltonian $H(q,p) = U(q) + \frac{1}{2}p^\top p$. Manifold $M = \{ q \in \mathbb{R}^m : g(q) = 0 \}$ embedded in $\mathbb{R}^m$ where $g : \mathbb{R}^m \to \mathbb{R}$. Jacobian of the constraint function $G : \mathbb{R}^m \to \mathbb{R}^{k \times m}$.
2: Initial position and momentum variables $q_0 \in M$ and $p_0 \in T^*_q M$. Integration step-size $\epsilon$ and number of integration steps $N \in \mathbb{N}$. Skew-symmetric matrix $L \in \mathbb{S}(m)$.
3: for $n = 0, \ldots, N - 1$ do
4: Compute $\mu$ using algorithm 4.
5: Compute $\tilde{p}_{n+1}/2$ using eq. (13).
6: Compute $(q_{n+1}, \tilde{p}_{n+1})$ using algorithm 2 with input $(q_n, \tilde{p}_{n+1}/2)$, step-size $\epsilon$, and $L$.
7: Use eq. (18) to compute $\mu'$.
8: Compute $p_{n+1}$ using eq. (16).
9: end for
10: Return: $(q_N, p_N)$.

The Lagrange multipliers $\mu$ and $\mu'$ are chosen such that eqs. (15) and (17) are satisfied. Such Lagrange multipliers exist, and are unique, provided $\epsilon \neq 0$ is small enough; see McLachlan et al. (2012). Note that when eqs. (15) and (17) are satisfied, $q_{n+1} \in M$ and $p_{n+1} \in T^* q_{n+1} M$ (for Hamiltonians of the form in eq. (6)) but that $\tilde{p}_{n+1}/2$ and $\tilde{p}_{n+1}$ are not guaranteed to respect the manifold constraint.

Pseudo-code for this manifold-constrained integrator corresponding to eqs. (13) to (17) is presented in algorithm 3. To prove the manifold integrator in algorithm 3 is symmetric and symplectic, we leverage lemma 2 to obtain the following result.

Theorem 3 (Symmetry and Symplecticness of Algorithm 3). The integration scheme in algorithm 3 is symplectic and symmetric.

A proof is given in appendix H. The order of algorithm 3 as an integrator of magnetic dynamics is derived in appendix I. Having constructed a symmetric and symplectic integrator on the manifold, we may apply algorithm 3 in algorithm 1 to yield a manifold-constrained magnetic HMC procedure.

Lagrange multipliers. In practice, the Lagrange multiplier $\mu$ is identified via Newton’s method. This procedure is summarized in algorithm 4. Note that the root of $f$ in algorithm 3 is a Lagrange multiplier satisfying eq. (15). The second Lagrange multiplier $\mu'$ may be obtained in closed-form by rearranging eqs. (16) and (17) and solving the normal equations

$$\frac{\epsilon}{2} G(q_{n+1}) G(q_{n+1})^\top \mu' = G(q_{n+1}) \tilde{p}_{n+1} + (18)$$

which has a unique solution when $G(q_{n+1})$ has full rank (recall $G$ is the Jacobian of the constraint).

6 EXPERIMENTS

In this section we give experimental evaluations of the magnetic manifold HMC sampler. We compare against three competing methods: (i) canonical HMC on the manifold, (ii) Metropolis-adjusted Langevin diffusions on the manifold, and (iii) random walk Metropolis on the manifold, all of which were implemented according to the description in Brubaker et al. (2012). The magnetic structure $L$ is a hyperparameter which we select by random search over five randomly-generated skew-symmetric matrices.
Table 1: Minimum expected sample size (Min.) and mean expected sample size (Mean) metrics and per-second timing comparisons for the linearly-constrained Gaussian task over ten independent trials.

| Method      | Min. | Mean | Min. / Sec. | Mean / Sec. |
|-------------|------|------|-------------|-------------|
| Metropolis  | 21.91| 239.88| 1,503.29 | 16,484.988 |
| Langevin    | 30.02| 1,517.12| 1,151.95 | 57,512.40 |
| Canonical   | 8,869.02| 9,717.35 | 21,001.408 | 89,347.71 |
| Magnetic    | 9,659.75| 9,914.93 | 20,768.29 | 97,093.14 |

Table 2: Minimum expected sample size (Min.) and mean expected sample size (Mean) metrics and per-second timing comparisons for the Bingham-von Mises-Fisher task over ten independent trials.

| Method      | Min. | Mean | Min. / Sec. | Mean / Sec. |
|-------------|------|------|-------------|-------------|
| Metropolis  | 370.013| 445.074 | 2,541.308 | 3,057.195 |
| Langevin    | 37,001.408| 21,001.408 | 89,347.71 |
| Canonical   | 10,000.0| 10,000.0 | 11,268.489 | 11,268.489 |
| Magnetic    | 9,909.768| 1,076.740 | 4,850.082 | 5,936.75 |

6.1 Gaussian Under Linear Constraints

Our first example considers sampling from a Gaussian distribution subject to linear constraints. Let \( g(q) = Ax - b \) for \( A \in \mathbb{R}^{m \times n} \) and \( b \in \mathbb{R}^m \). \( M = \{ g \in \mathbb{R}^m : g(q) = 0 \} \) is a linear submanifold of Euclidean space. We wish to draw samples from \( \text{Normal}(\mu, \Sigma | g(q) = 0) \). Following Brubaker et al. (2012) we set \( b = (0,0)^T \) and \( A = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & 1 \end{pmatrix} \) and set the parameters of the normal distribution to be \( \mu = (0, 0, 0, 0)^T \) and \( \Sigma = \text{diag}(1, 1, 1/100, 1/100) \). We initialize each sampler at the mode of the distribution, which corresponds with the Gaussian mean at \( \mu \). We sample 10,000 times from the target distribution and compute effective sample size statistics; we truncate the effective sample size at 10,000. We consider a grid search over possible parameters \( c \in \{1/10, 1/100, 1/1000\} \) and \( N \in \{5, 10, 100, 1000\} \) and compute the best-case performance of the samplers when results are averaged over ten independent trials. Results are shown in [table 1](#table1). The magnetic integrator achieved an ESS of over 10,000 in each of the six coefficients, outperforming the other three samplers on this task; HMC can exhibit ESS exceeding the number of samples if samples are negatively correlated.

6.2 Bingham-von Mises-Fisher Distribution

We next consider sampling from a Bingham-von Mises-Fisher distribution on \( \mathbb{S}^5 \subset \mathbb{R}^6 \). This distribution is defined by \( \pi(q) \propto \exp(b^T q + q^T A q) \) for \( b \in \mathbb{R}^6 \) and \( A \in \mathbb{R}^{6 \times 6} \). We randomly generate a square positive definite matrix \( A \) and standard normal vector \( b \) and compare the performance of the four manifold samplers we consider. As in the linearly-constrained Gaussian experiments, we sample 10,000 times from the target distribution and compute effective sample size statistics; we truncate the effective sample size at 10,000. We consider a grid search over possible parameters \( c \in \{1/10, 1/100, 1/1000\} \) and \( N \in \{5, 10, 100, 1000\} \) and compute the best-case performance of the samplers when results are averaged over ten independent trials. Results are shown in [table 2](#table2). The magnetic integrator achieved an ESS of over 10,000 in each of the six coefficients, outperforming the other three samplers on this task; HMC can exhibit ESS exceeding the number of samples if samples are negatively correlated.

6.3 Non-Conjugate Simplex Model

Denote the simplex embedded in \( \mathbb{R}^n \) by \( \Delta^{n-1} = \{ \theta \in \mathbb{R}^n : \theta \geq 0 \text{ and } \sum_i \theta_i = 1 \} \). We consider the volleyball dataset from Hankin (2019), which consists of nine volleyball players; each player has a skill \( \theta_i \) such that \( (\theta_1, \ldots, \theta_9) \in \Delta^n \). For each game, players are partitioned into teams \( T_1, T_2 \subset \{1, \ldots, 9\} \) and the probability that \( T_1 \) triumphs over \( T_2 \) in a game of volleyball is modeled as \( \sum_{i \in T_1} \theta_i / \sum_{i \in T_1 \cup T_2} \theta_i \). Given a Dirichlet prior \( \theta \sim \text{Dirichlet}(\alpha_1, \ldots, \alpha_9) \) and observations of teams and victories, the inference task is to sample from the posterior over \( \theta \). Because the simplex is not expressible as the zero levelset of some function (due the the positivity constraint), we follow Byrne and Girolami (2013) and embed the simplex into the positive orthant of \( \mathbb{S}^{n-1} \) by the mapping \( (q_1, \ldots, q_n) \mapsto (\sqrt{q_1}, \ldots, \sqrt{q_n}) \) and draw samples on \( \mathbb{S}^{n-1} \) instead of \( \Delta^{n-1} \); see Byrne and Girolami (2013) for full details. Samples on \( \mathbb{S}^{n-1} \) can be transformed back to \( \Delta^{n-1} \) by the map \( q_i \mapsto q_i^2 \). We set \( \epsilon = 0.01 \) and \( N = 20 \) in these experiments and consider \( \alpha_1 = \ldots = \alpha_9 = \alpha \) for \( \alpha \in \{1, 3, 5\} \). Results are summarized in [table 3](#table3) magnetic manifold HMC is strongest when an informative (\( \alpha > 1 \)) Dirichlet prior is used whereas canonical HMC performs better in the case of the non-informative prior \( \alpha = 1 \).

6.4 Network Eigenmodel

We consider Bayesian inference in the context of network analysis using the example from Byrne and Girolami (2013); Hoff (2009). This application considers protein interactions in a network of 230 proteins. Formally, the observations consist of a 230 \( \times 230 \) adjacency matrix \( \Delta \) whose \( (i,j) \) entry, \( \delta_{ij} \), equals one if the \( i^{th} \) and \( j^{th} \) proteins interact. Let \( \phi : \mathbb{R} \rightarrow (0,1) \) denote the probit function. The objective is to perform inference in the following Bayesian model:

\[
\delta_{ij} | U, \Sigma, c \sim \text{Bernoulli}(\phi((U \Sigma U^T)_{ij} + c))
\]
with priors $\sigma_i \sim \text{Normal}(0, 230)$, $c \sim \text{Normal}(0, 100)$, and $U \sim \text{Uniform}((\text{Stiefel}(230, 3))$, where $\Sigma = \text{diag}(\sigma_1, \sigma_2, \sigma_3)$ and $\text{Stiefel}(230, 3)$ is the Stiefel manifold consisting of $230 \times 3$ orthogonal matrices. This model is interpreted as identifying a low-rank eigendecomposition of a matrix whose probit transform models the probability of proteins interacting.

This is a challenging posterior for gradient-based Bayesian inference because it is multi-modal. To sample from all the modes of the distribution, it is necessary to combine multiple Markov chains with a parallel tempering scheme (Byrne and Girolami, 2013). This method permits HMC transitions to go between modes of the distribution. Our experiments instead consider the question of whether particular choices of magnetic structure influence which mode of the distribution magnetic manifold HMC will target. We therefore generated several magnetic structures by skew-symmetrizing a standard normal matrix and compared their mode-finding behavior.

We found that random walk Metropolis and manifold Langevin were ineffective in this task. Therefore, we restrict our discussion to the canonical and magnetic variants of HMC. Let $\Xi \text{diag}(\alpha) \Xi^\top$ be the rank-3 singular value decomposition of $\Delta$ where $\Xi \in \text{Stiefel}(230, 3)$ and $\alpha \in \mathbb{R}^3$. From the initial condition $c = 0$, $\sigma_i = \alpha_i$ for $i = 1, 2, 3$, and $U = \Xi$, canonical HMC regularly falls into one of two modes with potential values approximately 2,100 (smaller mode) and 1,900 (larger mode), a phenomenon previously observed in Byrne and Girolami (2013). Intriguingly, it is possible to prescribe magnetic structures which tend to target either of these modes, with virtually all sampling trajectories of magnetic HMC concentrating in one of the modes. Even more interesting is that there is a magnetic structure which sometimes targets a “rare mode” with potential value approximately 2,000 that canonical HMC never enters. All of these phenomena are illustrated across twenty random sampling trajectories in fig. 1. This phenomenon could be exploited for targeting modes in multi-modal distributions.

### 7 CONCLUSION

This paper presented the magnetic manifold HMC algorithm. We discussed the theory of magnetic Hamiltonian dynamics embedded in an ambient Euclidean space. We proved that these dynamics conserve energy and volume on the manifold. We proposed a symmetric and symplectic numerical integrator for these dynamics. We evaluated the magnetic manifold HMC procedure on manifold-constrained sampling tasks. Our experimental results show the promise of introducing magnetic effects into the proposal operator used in HMC. We defer to future work the study of how magnetic structures may be generated to explore the posterior and favor certain modalities.
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A Extended Preliminaries

This appendix is intended to provide preliminary mathematics, geometry, and physics for understanding the proofs. It is organized as a collection of definitions and facts which are referenced in the proofs where they are needed. Where possible, citations with page numbers are given for previously established facts.

A.1 General Mathematics

**Definition 23** (Permutation Group). Denote by $S^n$ the group of permutations on $n$ elements.

**Definition 24.** The sign of a permutation $\sigma \in S^n$, denoted $\text{sign}(\sigma)$, is the parity (+1 if even, −1 if odd) of the number of transpositions required to write the permutation.

**Definition 25** (Skew-Symmetric Matrix). A matrix $J$ is skew-symmetric if $J^T = -J$. The set of skew-symmetric $n \times n$ matrices is denoted $\text{Skew}(n)$.

**Fact 1** (Skew-Symmetric Matrices Annihilate Vectors). For a skew-symmetric matrix $J \in \text{Skew}(n)$ and a vector $x \in \mathbb{R}^n$, $x^T J x = 0$.

**Definition 26** (Skew-Symmetric Linear Map (Page 393 in Abraham et al. (1988))). Let $V$ be a vector space. A map $\alpha : V \times \cdots \times V \rightarrow \mathbb{R}$ ($k$ times) is skew-symmetric if

$$\alpha(v_1, \ldots, v_k) = \text{sign}(\sigma)\alpha(v_{\sigma(1)}, \ldots, v_{\sigma(k)})$$

where $\sigma \in S^k$ is a permutation.

**Fact 2** (Inverse Function Theorem). Let $f : \mathbb{R}^k \rightarrow \mathbb{R}^k$ be differentiable. Suppose that at $\mu \in \mathbb{R}^k$ the Jacobian $\nabla_{\mu} f(\mu)$ has non-zero determinant. Then there exists an open set $O$ containing $\mu$ such that there exists a differentiable inverse function $f^{-1} : f(O) \rightarrow O$.

A.2 Differential Forms

Differential forms are an important topic in differential geometry. Nearly any book on differential geometry will contain a detailed discussion of these objects. For instance, Abraham et al. (1988); Lee (2003); Marsden and Ratiu (2010) all contain detailed sections on differential forms.

**Definition 27** (Differential $k$-form (Page 129 of Marsden and Ratiu (2010))). Let $M$ be a manifold of dimension $m$ and let $q \in M$. A differential $k$-form $\alpha$ on $M$ ($k \leq m$) is a skew-symmetric linear map $\alpha : T_q M \times \cdots \times T_q M \rightarrow \mathbb{R}$ ($k$ times).

For a complete appreciation of our theoretical results, an understanding of 1-, 2-, and $m$-forms will be required. The most important 1-forms are the coordinate 1-forms.

**Definition 28** (Coordinate 1-Forms). Let $M$ be a manifold of dimension $m$ and let $q \in M$ with $q = (q_1, \ldots, q_m)$. The coordinate 1-forms are $dq_i : T_q M \rightarrow \mathbb{R}$ defined by $dq_i(v) = v_i$ where $v = (v_1, \ldots, v_m) \in T_q M$.

The wedge product of differential forms is the principle tool by which differential forms are combined to give another differential form.

**Definition 29** (Wedge Product). Let $\alpha$ be a differential $k$-form and $\beta$ a differential $l$-form. The wedge product of $\alpha$ and $\beta$, denoted $\alpha \wedge \beta$, is a $(k + l)$-form defined by

$$\left(\alpha \wedge \beta\right)(v_1, \ldots, v_{k+l}) \overset{\text{def}}{=} \frac{1}{k! l!} \sum_{\sigma \in S^{k+l}} \text{sign}(\sigma)\alpha(v_{\sigma(1)}, \ldots, v_{\sigma(k)})\beta(v_{\sigma(k+1)}, \ldots, v_{\sigma(k+l)})$$

where $S^{k+l}$ denotes the permutation group on $k + l$ elements.
**Fact 3** (Wedge Product of Coordinate 1-Forms). Let \( dq_i \) and \( dq_j \) be coordinate 1-forms. Let \( u, v \in T_q M \) with \( u = (u_1, \ldots, u_m) \) and \( v = (v_1, \ldots, v_m) \). Then
\[
(dq_i \wedge dq_j)(u, v) = u_i v_j - u_j v_i
\] (24)

*Proof.* Using definition \( ^{[28]} \) and the fact that the permutation group on two elements has only two elements, direct computation yields,
\[
(dq_i \wedge dq_j)(u, v) = \frac{1}{1!!} dq_i(u) dq_j(v) - dq_i(v) dq_j(u)
\] (25)
\[
= u_i v_j - v_i u_j
\] (26)
\[
= u_i v_j - u_j v_i.
\] (27)

**Fact 4** (\( k \)-Forms from Coordinate 1-Forms (Page 131 in Marsden and Ratiu (2010))). In terms of the coordinate 1-forms, any differential \( k \)-form may be written as
\[
\alpha = \sum_{i_1 < \cdots < i_k} \alpha_{i_1, \ldots, i_k}(q) \ dq_{i_1} \wedge \cdots \wedge dq_{i_k}
\] (28)
where \( \alpha_{i_1, \ldots, i_k} : M \to \mathbb{R} \) are smooth functions.

**Definition 30** (Constant Differential Form). A differential \( k \)-form is called constant when, for all \( i_1 < \cdots < i_k \), the \( \alpha_{i_1, \ldots, i_k} \) in fact \( \text{4} \) are all constant functions.

**Fact 5** (Wedge Product and Pullback (Page 131 in Marsden and Ratiu (2010))). Let \( \alpha \) be differential \( k \)-form and \( \beta \) be a differential 1-form on a manifold \( M \). Let \( \Phi : M \to \tilde{M} \) be a smooth function. Then,
\[
\Phi^*(\alpha \wedge \beta) = (\Phi^* \alpha) \wedge (\Phi^* \beta)
\] (29)

**Definition 31** (Non-Vanishing Differential Form). A differential \( k \)-form \( \alpha \) is said to be non-vanishing if for every \( q \in M \) there exists \( v_1, \ldots, v_k \in T_q M \) such that \( \alpha(v_1, \ldots, v_k) \neq 0 \).

**Definition 32** (Volume Form (Page 139 in Marsden and Ratiu (2010))). Given a manifold \( M \) of dimension \( m \), a nowhere vanishing differential \( m \)-form on \( M \) is called a volume form.

**Fact 6** (Dimension of Volume Forms (Page 399 in Abraham et al. (1988))). The vector space of all constant \( m \)-forms on \( \mathbb{R}^m \) is a vector space of dimension one.

**Definition 33** (Determinant). Let \( \Phi : M \to \tilde{M} \) be a smooth map and \( V \) a volume form on \( M \). Then \( \Phi^* V \) is another \( m \)-form on \( M \). The function \( \det(\Phi) : M \to \mathbb{R} \) such that
\[
\Phi^* V = \det(\Phi)V
\] (30)
is called the determinant of \( \Phi \).

**Fact 7** (Volume Preservation and Determinant (Page 140 in Marsden and Ratiu (2010))). A transformation \( \Phi \) is volume preserving for \( V \) if and only if \( \det(\Phi) = 1 \).

It will be convenient to work with vectors of differential 1-forms rather than individual 1-forms. The following definition extends the wedge product of differential 1-forms to vectors of differential 1-forms.

**Definition 34** (Wedge Product of Vectors of 1-Forms). Let \( da \) and \( db \) be \( m \)-dimensional vectors of differential 1-forms. For instance \( da = (da_1, \ldots, da_m) \). The wedge product of such vectors is defined by the relation
\[
da \wedge db \overset{\text{def}}{=} \sum_{i=1}^m da_i \wedge db_i
\] (31)

**Fact 8** (Properties of Wedge Product (Page 64 in Leimkuhler and Reich (2005))). Let \( da, db, dc \) be \( m \)-dimensional vectors of differential 1-forms. For instance \( da = (da_1, \ldots, da_m) \). The following are properties of the wedge product:
1. Skew-symmetry:

\[ da \wedge db = -db \wedge da \]  

(32)

2. Linearity:

\[ da \wedge (r \; db \wedge s \; dc) = r \; da \wedge db + s \; da \wedge dc \]  

(33)

for \( r, s \in \mathbb{R} \).

3. Matrix multiplication: For a matrix \( L \in \mathbb{R}^{m \times m} \),

\[ da \wedge L \; db = L^\top \; da \wedge db. \]  

(34)

4. Annihilation: When \( L \) is a symmetric matrix,

\[ da \wedge L \; da = 0. \]  

(35)

**Fact 9** (Differential 2-forms and Symplectic Structures). Let \( q = (q_1, \ldots, q_m) \in M \) and \( p = (p_1, \ldots, p_m) \in T^*_q M \) and set \( z = (q, p) \in T^* M \). A symplectic structure \( \Omega \) (see definition 7) with matrix \( J \in \text{Skew}(2m) \) may be written in terms of wedge products as

\[ \Omega = \sum_{i<j} J_{ij} \; dz_i \wedge dz_j \]  

(36)

\[ = \frac{1}{2} \; dz \wedge J \; dz \]  

(37)

**Proof.** Let \( u, v \in T_z T^* M \). The relation eq. (36) is standard and may be found in [Marsden and Ratiu (2010)] on page 147. To prove it, it suffices to use definition 28 and fact 3 which yields

\[ \sum_{i<j} J_{ij} \; dz_i \wedge dz_j(u, v) = \sum_{i<j} J_{ij} u_i v_j - J_{ij} u_j v_i \]  

(38)

\[ = \sum_{i<j} J_{ij} u_i v_j + J_{ji} u_j v_i \]  

(39)

\[ = \sum_{i=1}^{2m} \sum_{j=1}^{2m} J_{ij} u_i v_j \]  

(40)

\[ = u^\top \; J \; v \]  

(41)

\[ = \Omega(u, v) \]  

(42)

Equation (37) follows first from

\[ \sum_{i=1}^{2m} \sum_{j=1}^{2m} J_{ij} \; dz_i \wedge dz_j = \sum_{i<j} J_{ij} \; dz_i \wedge dz_j + J_{ji} \; dz_j \wedge dz_i \]  

(43)

\[ = \sum_{i<j} J_{ij} \; dz_i \wedge dz_j \]  

(44)

\[ = \sum_{i<j} J_{ij} \; dz_j \wedge dz_i \]  

(45)

\[ = \sum_{i<j} J_{ij} \; dz_i \wedge dz_j \]  

(46)

\[ = \sum_{i<j} 2 \; J_{ij} \; dz_i \wedge dz_j \]  

(47)
and, using definition 34 from

$$\sum_{i<j} J_{ij} dz_i \wedge dz_j = \frac{1}{2} \sum_{i=1}^{2m} \sum_{j=1}^{2m} J_{ij} dz_i \wedge dz_j$$

(48)

$$= \frac{1}{2} \sum_{i=1}^{2m} \sum_{j=1}^{2m} dz_i \wedge J_{ij} dz_j$$

(49)

$$= \frac{1}{2} \sum_{i=1}^{2m} dz_i \wedge \sum_{j=1}^{2m} J_{ij} dz_j$$

(50)

$$= \frac{1}{2} dz \wedge J dz$$

(51)

Fact 10 (Constant Symplectic Structure). The symplectic structures we consider are constant (see definition 30) since $J_{ij}$ does not depend on $z$.

Fact 11 (Magnetic Symplectic Structure). In the particular case corresponding to a magnetic symplectic structure we will have

$$J_{\text{mag}} = \begin{pmatrix} L & \text{Id}_m \\ -\text{Id}_m & 0_m \end{pmatrix} \in \text{Skew}(2m)$$

(52)

for some skew-symmetric matrix $L \in \mathbb{R}^{m \times m}$. Applying definition 34 and fact 9, the symplectic form can be expressed as

$$\sum_{i<j} J_{ij} dz_i \wedge dz_j = \sum_{i=1}^{n} dq_i \wedge dp_i + \sum_{i<j} L_{ij} dq_i \wedge dq_j$$

(53)

$$= dq \wedge dp + \frac{1}{2} dq \wedge L dq.$$  

(54)

Fact 12 (Magnetic Motion). For a Hamiltonian $H : \mathbb{R}^m \times \mathbb{R}^m \to \mathbb{R}$, the motion of $(q,p) \in \mathbb{R}^{2m}$ under a magnetic symplectic structure is given by

$$\dot{q} = \nabla_p H(q,p)$$

(55)

$$\dot{p} = -\nabla_q H(q,p) - L \nabla_p H(q,p)$$

(56)

Proof. Identify $z = (q,p)$. Given a magnetic symplectic structure with matrix,

$$J_{\text{mag}} = \begin{pmatrix} L & \text{Id}_m \\ -\text{Id}_m & 0_m \end{pmatrix}$$

(57)

for $L \in \text{Skew}(m)$, the Hamiltonian vector field $X_H$ is defined by

$$\Omega_{\text{mag}}(X_H(z), \delta) = \nabla_z H(z)^\top \delta$$

(58)

$$\implies X_H(z)^\top J_{\text{mag}} \delta = \nabla_z H(z)^\top \delta$$

(59)

$$\implies J_{\text{mag}}^\top X_H(z) = \nabla_z H(z)$$

(60)

$$\implies X_H(z) = (-J_{\text{mag}})^{-1} \nabla_z H(z)$$

(61)

where we have used that $J_{\text{mag}}$ is skew-symmetric and therefore satisfies $J_{\text{mag}}^\top = -J_{\text{mag}}$ from definition 25. Moreover, the inverse of $-J_{\text{mag}}$ is

$$(-J_{\text{mag}})^{-1} = \begin{pmatrix} 0_m & \text{Id}_m \\ -\text{Id}_m & -L \end{pmatrix}. $$

(62)

Therefore,

$$\begin{pmatrix} \dot{q} \\ \dot{p} \end{pmatrix} = \begin{pmatrix} 0_m & \text{Id}_m \\ -\text{Id}_m & -L \end{pmatrix} \begin{pmatrix} \nabla_q H(q,p) \\ \nabla_p H(q,p) \end{pmatrix}$$

(63)

is the Hamiltonian vector field.
An important volume form for Hamiltonian mechanics is the Liouville volume form, which is constructed from differential 2-forms.

**Definition 35** (Liouville Volume Form (Page 149 in Marsden and Ratiu (2010))). Let $M$ be a manifold of dimension $m$ and let $\Omega$ be a symplectic 2-form on $M$. The Liouville volume form on $T^*M$ is the $2m$-form defined by,

$$
\Lambda = \frac{(-1)^{m(m-1)/2}}{m!} \Omega \wedge \cdots \wedge \Omega \quad \text{(there are $m$ copies of $\Omega$ in the wedge products).}
$$

When $\Omega = \Omega_{\text{can}} = dq \wedge dp$, denote the Liouville volume form by $\Lambda_{\text{can}}$. The Liouville volume form $\Lambda_{\text{can}}(v_1, \ldots, v_{2m})$ with $v_i = (v_{i,1}, \ldots, v_{i,2m})$ is proportional to the determinant of the matrix whose $(i,j)$ entry is $v^j_i$, which, in turn, is the signed volume of parallelepiped spanned by the columns of that matrix.

**Definition 36** (Diffeomorphism of $T^*M$). Let $\Phi : T^*M \to T^*M$ be a smooth, invertible mapping. Then $\Phi$ is called a diffeomorphism of $T^*M$.

**Fact 13** (Differential Forms and Change-of-Variables (Page 62 in Leimkuhler and Reich (2005))). Let $M$ be a manifold of dimension $m$ with $z \in T^*M$. Let $dz$ be the vector of coordinate 1-forms; see definition 28. Let $\Phi$ be a smooth function and let $\hat{z} = \Phi(z)$. Then the coordinate 1-forms of $\hat{z}$ are transformations of the coordinate 1-forms of $z$:

$$
d\hat{z} = \sum_{j=1}^{2m} \frac{\partial \hat{z}_i}{\partial z_j} dz_j = \sum_{j=1}^{2m} \frac{\partial \Phi(z)_i}{\partial z_j} dz_j
$$

Or, letting $dz = (dz_1, \ldots, dz_{2m})$,

$$
d\hat{z} = \nabla_z \Phi(z)^\top dz
$$

where $\nabla_z \Phi(z)^\top$ is the Jacobian of $\Phi$.

**Fact 14** (Symplecticness and Differential 2-Forms). Let $\Omega$ be a symplectic structure with matrix $J$. A map $\Phi : T^*M \to T^*M$ is symplectic with respect to $\Omega$ if and only if

$$
\frac{1}{2} d\hat{z} \wedge J d\hat{z} = \frac{1}{2} dz \wedge J dz
$$

where $d\hat{z} = \nabla_z \Phi(z)^\top dz$.

**Proof.** A symplectic transformation is one that preserves the symplectic structure under pullback. If $\Phi : T^*M \to T^*M$ then

$$
(\Phi^* \Omega)(u, v) = \Omega((T_z \Phi)u, (T_z \Phi)v) = \Omega(u, v) \iff \Phi \text{ is symplectic}
$$

for all $u, v \in T_z T^*M$. Letting $u = (u_1, \ldots, u_{2m})$ and $v = (v_1, \ldots, v_{2m})$, in terms of the matrix $J$, this is nothing but

$$
(\nabla_z \Phi(z)^\top u)^\top J (\nabla_z \Phi(z)^\top v) = u^\top J v
$$

or

$$
\nabla_z \Phi(z) J \nabla_z \Phi(z)^\top = J.
$$

We can now establish that if $\hat{z} = \Phi(z)$ then symplecticness of $\Phi$ is equivalent to conservation of the 2-form. From fact 9, $\Omega$ can be written in terms of the wedge product as,

$$
\Omega = \frac{1}{2} dz \wedge J dz
$$
Using fact 13 under the change-of-variables $\dot{z} = \Phi(z)$, the symplectic structure changes to

$$\hat{\Omega} = \frac{1}{2} d\hat{z} \wedge \mathbb{J} d\hat{z}$$  (73)

$$= \frac{1}{2} \nabla_z \Phi(z)^\top d\hat{z} \wedge \mathbb{J} \nabla_z \Phi(z)^\top d\hat{z}. \quad (74)$$

Using fact 8,

$$\hat{\Omega} = \frac{1}{2} d\hat{z} \wedge \nabla_z \Phi(z) \mathbb{J} \nabla_z \Phi(z)^\top d\hat{z} \quad (75)$$

Hence we see that $\hat{\Omega} = \Omega$ when $\nabla_z \Phi(z) \mathbb{J} \nabla_z \Phi(z)^\top = \mathbb{J}$, which conforms with the definition of symplecticness.

**Fact 15** (Time Derivative and Symplecticness). Let $\Phi(\cdot;t) : T^*M \to T^*M$ be a smooth function. Let $\dot{z}_t = \Phi(z;t)$ be a change-of-variables given $z \in T^*M$ such that $z = \Phi(z;0)$. Let $\hat{\Omega}_t \overset{\text{def.}}{=} \frac{1}{2} d\hat{z}_t \wedge \mathbb{J} d\hat{z}_t$. Then $\Phi(\cdot;t)$ is symplectic with respect to $\Omega = \frac{1}{2} dz \wedge \mathbb{J} dz$ if $\frac{d}{dt} \hat{\Omega}_t = 0$.

**Proof.** By the fundamental theorem of calculus,

$$\hat{\Omega}_t - \hat{\Omega}_0 = \int_0^t \frac{d}{ds} \hat{\Omega}_s ds. \quad (76)$$

If $\frac{d}{dt} \hat{\Omega}_t = 0$ then

$$\hat{\Omega}_t = \hat{\Omega}_0. \quad (77)$$

Since $z_0 = z$, $\hat{\Omega}_t = \Omega$. The map $\Phi(\cdot;t)$ is symplectic by fact 14.

**A.3 Hamiltonian Dynamics**

**Fact 16** (Flow Property (Page 209 in Lee (2003))). Let $\Phi(\cdot;t)$ be a vector field flow to time $t$. Vector field flows satisfy the flow property:

$$\Phi(\Phi(q,p;t); -t) = (q,p) \quad (78)$$

or, equivalently,

$$\Phi(\cdot; -t) \circ \Phi(\cdot; t) = \text{Id} \quad (79)$$

**Fact 17** (Flows of Hamiltonian Vector Fields are Symplectic (Page 185 in Marsden and Ratiu (2010))). Let $\Phi(\cdot;t) : T^*M \to T^*M$ be the vector field flow (see definition 10) to time $t$ of a Hamiltonian vector field $X_H$ (see definition 9). Then $\Phi(\cdot;t)$ is symplectic for every $t$.

**Fact 18** (Composition of Symplectic Maps Form a Group (Page Page 72 in Marsden and Ratiu (2010))). Let $\Omega$ be a symplectic 2-form on $T^*M$. The collection of all maps $\Phi : T^*M \to T^*M$ such that $\Phi^*\Omega = \Omega$ forms a group under function composition.

**A.4 Embedded Geometry**

**Definition 37** (Embedded Cotangent Space). Let $H : \mathbb{R}^m \times \mathbb{R}^m \to \mathbb{R}$ be a smooth function. Let $M$ be manifold that can be embedded in $\mathbb{R}^m$ as the preimage of the zero level set of a constraint function $g : \mathbb{R}^m \to \mathbb{R}^k$; that is, let $M = \{ q \in \mathbb{R}^m : g(q) = 0 \}$. To view $T^*M$ as an embedded sub-manifold of $\mathbb{R}^{2m}$ means that $T^*M$ should be identified with the set

$$\{(q,p) \in \mathbb{R}^{2m} : g(q) = 0 \text{ and } G(q) \nabla_p H(q,p) = 0 \} \quad (80)$$

where $G(q) \in \mathbb{R}^{k \times m}$ is the Jacobian of the constraint function at $q$. 

Fact 19 (Velocity Constraint). View $T^*M$ as an embedded sub-manifold of $\mathbb{R}^{2m}$. Given the constraint $g(q) = 0$, we may differentiate this constraint with respect to time to obtain a constraint on the velocity. Namely,

$$\frac{d}{dt}g(q) = G(q)\dot{q} = 0. \quad (81)$$

Fact 20 (Velocity and Hamiltonian). In Hamiltonian mechanics, $\dot{q} = \nabla_p H(q,p)$. Hence, $G(q)\dot{q} = G(q)\nabla_p H(q,p) = 0$ is the constraint on $p$.

Fact 21 (Cotangent Space of Embedded Cotangent Bundle (Page 187 in Leimkuhler and Reich (2005))). View $T^*M$ as an embedded sub-manifold of $\mathbb{R}^{2m}$. The embedded cotangent space of $T^*M$, denoted $T^*T^*M$, is a subset of $T^*\mathbb{R}^{2m}$. Let $dq_1, \ldots, dq_m, dp_1, \ldots, dp_m \in T^*\mathbb{R}^{2m}$ be the coordinate 1-forms in the Euclidean space (see definition 28). The restriction of these differential 1-forms to $T^*T^*M$ implies that they satisfy,

$$G(q) \ dq = 0$$

$$f_q(q,p) \ dq + f_p(q,p) \ dp = 0,$$  \quad (82)

where $f(q,p) \equiv G(q)\nabla_p H(q,p)$ is the velocity constraint from facts 19 and 20 and $f_q(q,p)$ (resp. $f_p(q,p)$) represents its Jacobian with respect to $q$ (resp. $p$).

Fact 22 (Wedge Product with Lagrange Multipliers Vanish (Page 187 in Leimkuhler and Reich (2005))). Let $q \in \mathbb{R}^n$. Let $g : \mathbb{R}^n \to \mathbb{R}^k$ be the constraint function with Jacobian $G(q) \in \mathbb{R}^{k \times n}$. Suppose $g(q) = 0$. Then for any $\mu \in \mathbb{R}^k$,

$$dq \wedge d(G(q)^\top \mu) = 0 \quad (84)$$

Proof. We have

$$dq \wedge d(G(q)^\top \mu) = dq \wedge G(q)^\top d\mu + \sum_{i=1}^{k} dq \wedge \mu_i \Gamma_i dq = 0,$$  \quad (85)

where $\Gamma_i$ is the Hessian of the $i$th constraint function. By symmetry of the Hessian and eq. (35) from fact 8, the second term is zero. The first term is also zero because $g(q) = 0 \implies G(q)dq = 0$ and since $dq \wedge G(q)\ d\mu = G(q)dq \wedge d\mu = 0$. \qed

A.5 Physics

Fact 23 (Total Force). The total force acting on an object is the sum of all individual forces.

Fact 24 (D’Alembert’s Principle). Constraint forces act in the normal direction to the constraint surface. Given a constraint function $g : \mathbb{R}^n \to \mathbb{R}^k$, constraint forces are therefore represented by $-G(q)^\top \lambda$ for $\lambda \in \mathbb{R}^k$.

Fact 25 (Lorentz Force Law). The force on a particle $q \in \mathbb{R}^3$ under the influence of a magnetic field is given by $m \times \frac{1}{m} q$ where $m \in \mathbb{R}^3$ represents parameters of the magnetic field and $\times$ is the vector cross-product; that is,

$$m \times \frac{d}{dt}q = \begin{pmatrix} 0 & m_1 & -m_2 \\ -m_1 & 0 & m_3 \\ m_2 & -m_3 & 0 \end{pmatrix} \begin{pmatrix} \dot{q}_1 \\ \dot{q}_2 \\ \dot{q}_3 \end{pmatrix} \quad (86)$$

A.6 Numerical Integration

Definition 38 (Order of Integration). Let $\hat{\Phi}(\cdot;\epsilon,1) : T^*M \to T^*M$ be a single step numerical integrator (definition 12) for the Hamiltonian vector field flow $\Phi(\cdot;\epsilon) : T^*M \to T^*M$ (definition 10). Then $\hat{\Phi}$ is said to have order $k \in \mathbb{N}$ if for any $(q,p) \in T^*M$ we have

$$\hat{\Phi}((q,p);\epsilon,1) - \Phi((q,p);\epsilon) = \mathcal{O}(\epsilon^{k+1}) \quad (87)$$

Fact 26 (Symmetric Order of Integration (Page 86 in Leimkuhler and Reich (2005))). Let $\hat{\Phi}(\cdot;\epsilon,1) : T^*M \to T^*M$ be a single step numerical integrator (definition 12) for the Hamiltonian vector field flow $\Phi(\cdot;\epsilon) : T^*M \to T^*M$ (definition 10). Suppose further that $\hat{\Phi}$ is a symmetric integrator (definition 14). Then the order of $\hat{\Phi}$ is even.
B  Physical Interpretation of Motion

This result requires facts 23, 24 and 25.

Lemma. Let \( M = \{ q \in \mathbb{R}^3 : g(q) = 0 \} \) be a manifold such that \( G(q) \) has full-rank. Consider a Hamiltonian of the form \( H(q,p) = U(q) + \frac{1}{2}p^T B p \) with \( (q,p) \in T^* M \) and \( b \in \mathbb{R}_+ \). Then the equations of motion in eqs. (10) to (12) correspond to the motion of a particle, with mass \( b \), simultaneously undergoing potential, magnetic, and manifold constraint forces.

Proof. It is common to express potential forces as the negative gradient of some function \( U : \mathbb{R}^3 \to \mathbb{R} \) called the potential function. The Hamiltonian equations of motion for \( H(q,p) \) with a magnetic symplectic structure \( \Omega_{\text{mag}} \) are:

\[
\dot{q}_t = \frac{p_t}{b} \\
\dot{p}_t = -\nabla_q U(q_t) - L_{p_t} - G(q_t)^T \lambda \\
g(q_t) = 0
\]

(88)  (89)  (90)

Now noting that the momentum variables \( p_t = b \dot{q}_t \) by substitution we obtain,

\[
\dot{q}_t = \dot{q}_t \\
\dot{b} \dot{q}_t = -\nabla_q U(q_t) + m \times \dot{q}_t + G(q_t)^T (-\lambda)
\]

(91)  (92)

where, since \( L \) is a skew-symmetric matrix, we have used fact 25 to identify

\[
-L = \begin{pmatrix}
0 & m_1 & -m_2 \\
-m_1 & 0 & m_3 \\
m_2 & -m_3 & 0
\end{pmatrix}.
\]

(93)

We have used fact 24 to identify constraint forces and fact 23 to recognize that the sum of these three forces is the total force acting on the particle. Thus we see, by Newton’s second law of motion, that the Hamiltonian equations of motion are equivalent to Newtonian mechanics describing a particle subject to potential, magnetic, and constraint forces.
C Embedded Manifold Examples

Example 2 (Euclidean Space). Consider $\mathbb{R}^m$ which may degenerately be regarded as an embedded manifold whose constraint function is $g(q) = 0$ for all $q \in \mathbb{R}^m$ (i.e., the euclidean space, unconstrained). The Jacobian of the constraint is the $1 \times m$ vector of zeros, which is evidently not full-rank. Nevertheless, continuing the development shows that, for instance, $T_q\mathbb{R}^m = T^*_q\mathbb{R}^m = \mathbb{R}^m$ and $T^*\mathbb{R}^m = \mathbb{R}^m \times \mathbb{R}^m \cong \mathbb{R}^{2m}$.

Example 3 (The Sphere). As a second example, consider $\mathbb{S}^2$, the sphere, embedded in $\mathbb{R}^3$ as the preimage of the constraint function $g(q) = q^\top q - 1$ on the zero level set. The Jacobian of the constraint at $q \in \mathbb{S}^2$ is $G(q) = 2q^\top$ which has full-rank as a $1 \times 3$ matrix. The tangent space at $q \in \mathbb{S}^2$ is $T_q\mathbb{S}^2 = \{\xi \in \mathbb{R}^3 : 2q^\top \xi = 0\}$, the set of vectors orthogonal to $q$. Let $R$ be a $3 \times 3$ rotation matrix; an example of a mapping from $\mathbb{S}^2 \to \mathbb{S}^2$ is $\Phi(q) = Rq$, the rotation of $q$ by $R$. In this case, $T_q\Phi = R$ so that $(T_q\Phi)\xi = R\xi$, the rotation of the tangent vector by $R$. 


Comparison of Magnetic Geodesics

To give intuition for the motion generated by manifold-constrained magnetic Hamiltonian dynamics, we consider the motion of a particle under a Hamiltonian consisting purely of kinetic energy: \( H(q, p) = \frac{1}{2}p^\top p \). In the case of canonical dynamics, motion in \( q \) generated by this Hamiltonian can be shown to produce geodesic movement on a manifold (Marsden and Ratiu, 2010); that is, motion for which the particle experiences zero acceleration on the manifold. When a magnetic field is introduced, the resulting motion in \( q \) is called a “magnetic geodesic.”

We visualize the magnetic geodesic for a randomly generated \( L \) in \( \mathbb{R}^3 \), the sphere, and the special orthogonal group in fig. 2. Whereas the Euclidean geodesic is a straight line, the magnetic geodesic proceeds in a helix. On the sphere, the geodesic corresponds to great circles. The magnetic geodesic on the sphere is much more complicated, visiting many distinct regions of the sphere compared to the usual geodesic which returns to its initial position. We visualize a magnetic geodesic on \( \text{SO}(3) \) via its action on the vector \((1, 1, 1)^\top\). The action of the usual geodesic causes the vector to move about in a circle. The magnetic geodesic yields a more unusual and complicated motion of this vector.

We also illustrate that our integrator is reversible under applying a sign flip to the integration step-size \( \epsilon \mapsto -\epsilon \). These reverse trajectories have initial condition equal to the terminal condition of the forward trajectory and are integrated for the same number of integration steps with the reversed step-size. We see that in every case the reverse trajectory proceeds backwards along the magnetic geodesic, demonstrating symmetry of the integrator.
Proof of Theorem 4

This result requires facts [13, 20] and [21] and definitions [28] and [37].

**Theorem 4.** Let \( M = \{ q \in \mathbb{R}^m : g(q) = 0 \} \) be a connected manifold such that \( G(q) \) has full-rank. Let \( T^* M \) be an embedded sub-manifold of \( \mathbb{R}^{2m} \) as in definition [4]. Let \( \Omega_{mag} \) be the magnetic symplectic structure from definition [27] in the ambient Euclidean space \( \mathbb{R}^{2m} \cong \mathbb{R}^m \times \mathbb{R}^m \). Let \( H(q,p) \) be a smooth Hamiltonian \( H : \mathbb{R}^m \times \mathbb{R}^m \to \mathbb{R} \) of the form in eq. [4]. Let \( \Phi_{mag} \) be the magnetic vector field flow from definition [22]. Let \( (q_t, p_t) = \Phi_{mag}(q,p); t \). Then the embedded differential one-forms \( dq_t \) and \( dp_t \) respect the manifold constraints such that \( (dq_t, dp_t) \) are elements of \( T^* (q_t, p_t) M \).

In proving these results we will adopt the shorthand notation \( H_q \) to denote the partial derivative of \( H \) with respect to \( q \) regarded as a row vector. The notation \( H_{qp} \) denotes the matrix of partial derivatives of \( H \) with respect to \( q \) and \( p \). Other quantities similarly defined.

We will require preliminary lemmas before proving the theorems.

**Lemma 2.** For Hamiltonians of the form in eq. [0],
\[
H_{qp}(q,p) = H_{pq}(q,p) = 0
\]

**Proof.** The Hamiltonian is separable so that the potential energy \( U(q) \) is a function of \( q \) alone and the kinetic energy \( K(p) = \frac{1}{2} p^T p \) is a function of \( p \) alone. Differentiating with respect to \( q \) and then with respect to \( p \), or with respect to \( p \) and then with respect to \( q \) causes all terms to vanish.

**Lemma 3.** Given the constraint \( g(q_t) = 0 \), the differential \( dq_t \) must obey \( G(q_t) dq_t = 0 \).

**Proof.** Applying fact [13]
\[
d(g(q_t)) = d0 = 0 \implies G(q_t) dq_t = 0
\]

**Lemma 4.**
\[
d\dot{q}_t = H_{qp}(q_t, p_t) dq_t + H_{pp}(q_t, p_t) dp_t
\]
\[
d\dot{p}_t = -H_{qq}(q_t, p_t) dq_t - H_{qp}(q_t, p_t) dp_t - LH_{pq}(q_t, p_t) dq_t - LH_{pp}(q_t, p_t) dp_t - d(G(q_t)^T \lambda)
\]

**Proof.** The equations of motion are
\[
\dot{q}_t = \nabla_p H(q_t, p_t)
\]
\[
\dot{p}_t = -\nabla_q H(q_t, p_t) - L \nabla_p H(q_t, p_t) - G(q_t)^T \lambda
\]
\[
g(q_t) = 0
\]

Computing the differential yields,
\[
d\dot{q}_t = H_{pq}(q_t, p_t) dq_t + H_{pp}(q_t, p_t) dp_t
\]
\[
d\dot{p}_t = -H_{qq}(q_t, p_t) dq_t - H_{qp}(q_t, p_t) dp_t - LH_{pq}(q_t, p_t) dq_t - LH_{pp}(q_t, p_t) dp_t - d(G(q_t)^T \lambda)
\]

We may now prove theorem [4]

**Proof.** We want to show that the magnetic Hamiltonian dynamics
\[
\dot{q}_t = \nabla_p H(q_t, p_t)
\]
\[
\dot{p}_t = -\nabla_q H(q_t, p_t) - L \nabla_p H(q_t, p_t) - G(q_t)^T \lambda
\]
\[
0 = g(q_t)
\]
have the property that the embedded differential one-forms $dq$ and $dp$ satisfy the manifold constraints such that $(dq, dp)$ are elements of the cotangent space of the manifold $T^*T^*M$ viewed as an embedded submanifold of $T^*\mathbb{R}^{2m}$. From fact 21, this is equivalent to verifying that the solution to the magnetic Hamiltonian dynamics obey:

\begin{align}
G(q_t) \ dq_t &= 0 \\
f_q(q_t, p_t) \ dq_t + f_p(q_t, p_t) \ dp_t &= 0, 
\end{align}

where $f(q, p) \overset{\text{def}}{=} G(q) \nabla_p H(q, p)$. Applying lemma 3 immediately gives the first condition. The second condition follows from computing the time-derivative of $G(q_t) \ dq_t = 0$:

\begin{align}
\frac{d}{dt} [G(q_t) dq_t] &= \left[ \frac{d}{dt} G(q_t) \right] dq_t + G(q_t) d\dot{q}_t \\
&= [\nabla G(q_t) \cdot \dot{q}_t] \ dq_t + G(q_t) d\dot{q}_t \\
&= 0
\end{align}

Using fact 20 and lemma 2 computing the differentials of $f(q, p)$ yields

\begin{align}
f_q(q_t, p_t) \ dq_t &= [\nabla G(q_t) \cdot \dot{q}_t + G(q_t) H_{pq}(q_t, p_t)] \ dq_t \\
&= \left[ \nabla G(q_t) \cdot \dot{q}_t \right] \ dq_t \\
f_p(q_t, p_t) \ dp_t &= G(q_t) H_{pp}(q_t, p_t) \ dp_t
\end{align}

Using lemmas 2 and 4 the differential of eq. (104) gives the relation

\begin{align}
d\dot{q}_t &= H_{pq}(q_t, p_t) \ dq_t + H_{pp}(q_t, p_t) \ dp_t \\
\Rightarrow d\dot{q}_t &= H_{pp}(q_t, p_t) \ dp_t
\end{align}

whereupon substitution into eq. (114) yields,

\begin{align}
f_p(q_t, p_t) \ dp_t &= G(q_t) d\dot{q}_t
\end{align}

Therefore,

\begin{align}
f_q(q_t, p_t) \ dq_t + f_p(q_t, p_t) \ dp_t &= [\nabla G(q_t) \cdot \dot{q}_t] \ dq_t + G(q_t) d\dot{q}_t \\
&= 0
\end{align}

from eq. (111).
F Proof of Theorem 2

This result requires definitions 28, 34 and 37, facts 1, 8, 9, 11, 15, 16, 19, 20 and 22, and lemma 4.

Theorem. Let \( M = \{ q \in \mathbb{R}^m : g(q) = 0 \} \) be a connected manifold such that \( G(q) \) has full-rank. Let \( T^* M \) be an embedded sub-manifold of \( \mathbb{R}^{2m} \) as in definition 4. Let \( \Omega_{\text{mag}} \) be the magnetic symplectic structure from definition 21 in the ambient Euclidean space \( \mathbb{R}^{2m} \cong \mathbb{R}^m \times \mathbb{R}^m \). Let \( H(q,p) \) be a smooth Hamiltonian \( H : \mathbb{R}^m \times \mathbb{R}^m \to \mathbb{R} \) of the form in eq. (6). Let \( \Phi_{\text{mag}} \) be the magnetic vector field flow from definition 22. Then

\begin{enumerate}[label=(\roman*)]
  \item \( \Phi_{\text{mag}} \) is a symmetric map (definition 13): \( \Phi_{\text{mag}}(\Phi_{\text{mag}}(q,p; t); -t) = (q,p) \).
  \item \( \Phi_{\text{mag}}(\cdot ; t) \) is a symplectic transformation (definition 8) on \( T^* M : \Phi_{\text{mag}}^* \Omega_{\text{mag}} = \Omega_{\text{mag}} \).
  \item \( \Phi_{\text{mag}}(\cdot ; t) \) conserves the Hamiltonian: \( H(\Phi_{\text{mag}}(q,p; t)) = H(q,p) \) for any \( (q,p) \in T^* M \).
\end{enumerate}

There are three statements. First that the magnetic vector field flow is symmetric, second that it is symplectic, and third that it conserves the Hamiltonian. We will prove the three individually.

Lemma 5. Let \( M = \{ q \in \mathbb{R}^m : g(q) = 0 \} \) be a connected manifold such that \( G(q) \) has full-rank. View \( T^* M \) as an embedded sub-manifold of \( \mathbb{R}^{2m} \). Let \( \Omega_{\text{mag}} \) be the magnetic symplectic structure in the ambient Euclidean space \( \mathbb{R}^{2m} \cong \mathbb{R}^m \times \mathbb{R}^m \). Let \( H(q,p) \) be a smooth Hamiltonian \( H : \mathbb{R}^m \times \mathbb{R}^m \to \mathbb{R} \) of the form in eq. (6). Then \( \Phi_{\text{mag}} \) is symmetric: \( \Phi_{\text{mag}}(\Phi_{\text{mag}}(q,p; t); -t) = (q,p) \).

Proof. The map \( \Phi_{\text{mag}} : T^* M \to T^* M \) is a vector field flow by definition (see definition 22). By eq. (78) in fact 16, it is symmetric.

Lemma 6. Let \( M = \{ q \in \mathbb{R}^m : g(q) = 0 \} \) be a connected manifold such that \( G(q) \) has full-rank. View \( T^* M \) as an embedded sub-manifold of \( \mathbb{R}^{2m} \). Let \( \Omega_{\text{mag}} \) be the magnetic symplectic structure in the ambient Euclidean space \( \mathbb{R}^{2m} \cong \mathbb{R}^m \times \mathbb{R}^m \). Let \( H(q,p) \) be a smooth Hamiltonian \( H : \mathbb{R}^m \times \mathbb{R}^m \to \mathbb{R} \) of the form in eq. (6). Then \( \Phi_{\text{mag}}(\cdot ; t) \) is a symplectic transformation (definition 8) on \( T^* M \) for any \( t \).

Proof. We want to show that \( \Phi_{\text{mag}} \) is a symplectic transformation (definition 8). By fact 11, the magnetic symplectic structure can be written in terms of the wedge product as

\[
dq \wedge dp + \frac{1}{2} dq \wedge L dq
\]

from eq. (54). Let \( (q,p) = \Phi_{\text{mag}}(q,p; t) \). Denote \( \Omega_{\text{mag}}^t = dq_t \wedge dp_t + \frac{1}{2} dq_t \wedge L dq_t \). From fact 15, \( \Phi_{\text{mag}} \) is symplectic for the magnetic 2-form \( \Omega_{\text{mag}} \) if

\[
\frac{d}{dt} \Omega_{\text{mag}}^t = 0.
\]

Hence, our proof strategy will establish \( \frac{d}{dt} \Omega_{\text{mag}}^t = 0 \) which will imply that \( \Phi_{\text{mag}} \) is symplectic.

We use the differentials computed in lemma 4. The notation \( H_{qp} \) denotes the matrix of partial derivatives of \( H \) with respect to \( q \) and \( p \). Symmetry of partial derivatives yields \( H_{pq} = H_{qp}^\top \). The Hessian matrix with respect to \( q \) (resp. \( p \)) is denoted \( H_{qq} \) (resp. \( H_{pp} \)).

Computing the time derivative of \( \Omega_{\text{mag}}^t \), we have that the magnetic symplectic form is preserved under the
solution to the constrained system.

\[
\frac{d}{dt} \Omega_{\text{mag}} = dq_t \wedge dp_t + dq_t \wedge dp_t + \frac{1}{2} dq_t \wedge L dq_t + \frac{1}{2} dq_t \wedge L dq_t \tag{122}
\]

\[
= dq_t \wedge dp_t + dq_t \wedge dp_t + dq_t \wedge L dq_t \tag{123}
\]

\[
= H_{pq} dq_t \wedge dp_t + H_{pp} dp_t \wedge dp_t
\]

\[
- dq_t \wedge H_{qp} dq_t - dq_t \wedge L H_{pq} dq_t
\]

\[
- dq_t \wedge L H_{pp} dp_t - dq_t \wedge \text{d}(G(q_t)^\top \lambda)
\]

\[
+ H_{pq} dq_t \wedge L dq_t + H_{pq} dp_t \wedge L dq_t \tag{124}
\]

\[
= H_{pq} dq_t \wedge dp_t - H_{pq} dq_t \wedge dp_t
\]

\[
- dq_t \wedge L H_{pq} dq_t - L H_{pq} dp_t \wedge dq_t
\]

\[
- dq_t \wedge L H_{pp} dp_t - L H_{pp} dp_t \wedge dq_t
\]

\[
- dq_t \wedge \text{d}(G(q_t)^\top \lambda)
\]

\[
= 0 \tag{125}
\]

The final equality comes from manipulations of the wedge product using fact 8 and using the fact that \( L \) is a skew-symmetric matrix; in particular, we use eqs. (32), (34) and (35). That \( dq_t \wedge \text{d}(G(q_t)^\top \lambda) = 0 \) from fact 22.

**Lemma 7.** Let \( M = \{ q \in \mathbb{R}^m : g(q) = 0 \} \) be a connected manifold such that \( G(q) \) has full-rank. View \( T^* M \) as an embedded submanifold of \( \mathbb{R}^{2m} \). Let \( \Omega_{\text{mag}} \) be the magnetic symplectic structure in the ambient Euclidean space \( \mathbb{R}^{2m} \cong \mathbb{R}^m \times \mathbb{R}^m \). Let \( H(q,p) \) be a smooth Hamiltonian \( H : \mathbb{R}^m \times \mathbb{R}^m \rightarrow \mathbb{R} \) of the form in eq. (6). Then \( H(\Phi_{\text{mag}}(q,p;t)) = H(q,p) \) for any \( (q,p) \in T^* M \) so that the Hamiltonian energy is conserved.

**Proof.** Let \( (q_t,p_t) = \Phi_{\text{mag}}(q,p;t) \). To prove that the Hamiltonian is conserved, we verify that the time derivative of \( H(q_t,p_t) \) equals zero.

\[
\frac{d}{dt} H(q_t,p_t) = \nabla_q H(q_t,p_t) \cdot \dot{q}_t + \nabla_p H(q_t,p_t) \cdot \dot{p}_t \tag{128}
\]

\[
= \nabla_q H(q_t,p_t) \cdot L_p H(q_t,p_t) - \nabla_p H(q_t,p_t) \cdot \nabla_q H(q_t,p_t) + L \nabla_p H(q_t,p_t) + G(q_t)^\top \lambda
\]

\[
= -\nabla_p H(q_t,p_t) \cdot L \nabla_q H(q_t,p_t) - \nabla_p H(q_t,p_t) \cdot G(q_t)^\top \lambda \tag{129}
\]

\[
= 0 \tag{130}
\]

by fact 7 using that \( L \) is skew-symmetric and since \( G(q_t) \nabla_p H(q_t,p_t) = G(q_t)p_t = 0 \) from facts 19 and 20.

Therefore, by the Fundamental Theorem of Calculus:

\[
H(q_t,p_t) - H(q_0,p_0) = \int_0^t \frac{d}{ds} H(q_s,p_s) \, ds = 0. \tag{132}
\]

Therefore \( H(q_t,p_t) = H(q_0,p_0) \) and since \( (q_0,p_0) = (q,p) \) we have shown that \( H(q_t,p_t) = H(q,p) \).

We now give a proof of theorem 2.

**Proof.** Apply lemmas 5, 6 and 7. \( \square \)
G Proof of Lemma 1

This result requires facts 12, 16, 17, and 18.

Lemma (Symmetry and Symplecticness of Algorithm 2). The single-step integrator for magnetic dynamics in Euclidean space in algorithm 2 is symmetric and symplectic.

The magnetic integrator for Euclidean spaces is derived as the symmetric composition of three magnetic Hamiltonian vector field flows (definition 22). Consider a Hamiltonian of the form \( H(q,p) = U(q) + \frac{1}{2}p^\top p \). The integrator is derived from a Strang splitting of the Hamiltonian

\[
H(q,p) = \frac{1}{2}U(q) + \frac{1}{2}p^\top p + \frac{1}{2}U(q)
\]

(133)

The complete algorithm is given in algorithm 2.

The following lemmas are proved in Tripuraneni et al. (2017). They can both be derived from the motion established in eq. (63) from fact 12.

Lemma 8. Let \((q_0,p_0) \in \mathbb{R}^{2m}\). Denote the magnetic vector field flow (definition 22) to time \( \epsilon \) of \( H_1 \) under a magnetic symplectic structure by \( \Phi_1^\epsilon(\cdot,\cdot) : \mathbb{R}^{2m} \to \mathbb{R}^{2m} \). Then

\[
\Phi_1^\epsilon(q_0,p_0) = (q_0,p_0 - \epsilon/2 \cdot \nabla U(q_0)).
\]

Lemma 9. Let \((q_0,p_0) \in \mathbb{R}^{2m}\). Denote the magnetic vector field flow (definition 22) to time \( \epsilon \) of \( H_2 \) under a magnetic symplectic structure by \( \Phi_2^\epsilon(\cdot,\cdot; L) : \mathbb{R}^{2m} \to \mathbb{R}^{2m} \). Then \( \Phi_2^\epsilon \) has a closed-form expression given by

\[
(q',p') = \Phi_2^\epsilon(q,p; L)
\]

(135)

where

\[
p' \overset{\text{def.}}{=} \exp(-\epsilon L)p
\]

(136)

\[
q' \overset{\text{def.}}{=} q + (U_D \ U_0) \begin{pmatrix} D^{-1}(\exp(\epsilon D) - \Id) & 0 \\ 0 & \epsilon \Id \end{pmatrix} (U_D \ U_0)^{-1} p
\]

(137)

where

\[
-L = (U_D \ U_0) \begin{pmatrix} D & 0 \\ 0 & 0 \end{pmatrix} (U_D \ U_0)^{-1}
\]

(138)

is an eigen-decomposition of \(-L\) so that \(D\) is the diagonal matrix of non-zero eigenvalues, \(U_D\) is the matrix of eigenvectors for the non-zero eigenvalues, and \(U_0\) is the matrix of eigenvectors for the zero eigenvalues.

We will now prove lemma 1. This was already proven in Tripuraneni et al. (2017). Here we offer an alternative proof. There are two statements: (i) that the integrator is symmetric and (ii) that the integrator is symplectic. We will prove each individually.

Lemma 10. The single-step integrator in algorithm 2 is symmetric.

Proof. A single step of the numerical integrator is the symmetric composition of Hamiltonian flows for three sub-Hamiltonians; that is, it is the composition

\[
\hat{\Phi}(\cdot; \epsilon) \overset{\text{def.}}{=} \Phi_1^\epsilon \circ \Phi_2^\epsilon \circ \Phi_1^\epsilon : \mathbb{R}^{2m} \to \mathbb{R}^{2m},
\]

(139)

where \( \Phi_1^\epsilon \) is the magnetic Hamiltonian vector field flow defined in lemma 8 and \( \Phi_2^\epsilon \) is the magnetic Hamiltonian vector field flow defined in lemma 9. Because the composition is symmetric, it is reversible under negation of the step-size \( \epsilon \mapsto -\epsilon \) by the flow property of differential equations from fact 16 using eq. (79):

\[
\hat{\Phi}(\cdot; -\epsilon) \circ \hat{\Phi}(\cdot; \epsilon) = \Phi_1^{-\epsilon} \circ \Phi_2^{-\epsilon} \circ \Phi_1^{-\epsilon} \circ \Phi_2^\epsilon \circ \Phi_1^\epsilon
\]

(140)

\[
= \Phi_1^{-\epsilon} \circ \Phi_2^\epsilon \circ \Phi_1^\epsilon
\]

(141)

\[
= \Phi_1^{-\epsilon} \circ \Phi_1^\epsilon
\]

(142)

\[
= \Id.
\]

(143)
Lemma 11. The single-step integrator in algorithm 2 is symplectic.

Proof. A single step of the numerical integrator is the symmetric composition of Hamiltonian flows for three sub-Hamiltonians; that is, it is the composition

$$\hat{\Phi}(\cdot; \epsilon) \overset{\text{def}}{=} \Phi_{\epsilon}^1 \circ \Phi_{\epsilon}^2 \circ \Phi_{\epsilon}^3. \quad (144)$$

where $\Phi_{\epsilon}^1$ is the magnetic Hamiltonian vector field flow defined in lemma 8 and $\Phi_{\epsilon}^2$ is the magnetic Hamiltonian vector field flow defined in lemma 9. Hamiltonian flows are symplectic from fact 17 and form a group under composition from fact 18. Therefore, the integrator, which is a composition of three Hamiltonian flows, is symplectic.

We now give the proof of lemma 1.

Proof. Apply lemmas 10 and 11.
Proof of Theorem 3

This result requires lemma 1, facts 2, 11, 14, and 22, and definition 37.

Theorem (Symmetry and Symplecticness of Algorithm 3). The integration scheme in algorithm 3 is symplectic and symmetric.

To prove this theorem, we’ll first establish several related lemmas. The first result is a quick verification that the integrator is constrained to the manifold.

Lemma 12. Let \( M = \{ q \in \mathbb{R}^m : g(q) = 0 \} \) be a connected manifold such that \( G(q) \) has full-rank. Let \( T^*M \) be an embedded sub-manifold of \( \mathbb{R}^{2m} \) as in definition 4. Let \( \mu \) and \( \mu' \) be Lagrange multipliers such that eqs. (15) and (17) are satisfied. Then algorithm 3 maps \( (q_n, p_n) \in T^*M \) to \( (q_{n+1}, p_{n+1}) \in T^*M \).

Proof. Recall that \( M = g^{-1}(0) \) so that \( q \in M \iff g(q) = 0 \). If \( \mu \) is a Lagrange multiplier such that eq. (15) is satisfied, it is immediate that \( q_{n+1} \in M \). From definition 2, \( p \in T_q^*M \iff G(q)\nabla_p H(q, p) = 0 \). For Hamiltonians in the form of eq. (6), \( \nabla_p H(q, p) = p \) so that \( p \in T_q^*M \iff G(q)p = 0 \). If \( \mu' \) is a Lagrange multiplier satisfying eq. (17), then it is immediate that \( p_{n+1} \in T^*_{q_{n+1}}M \). Thus, by definition 4, \( (q_{n+1}, p_{n+1}) \in T^*M \).

Lemma 13. Let \( g : \mathbb{R}^m \to \mathbb{R}^k \) be a constraint function with full-rank Jacobian \( G : \mathbb{R}^m \to \mathbb{R}^{k \times m} \). Let \( q_n \in \mathbb{R}^m \) satisfy \( g(q_n) = 0 \) and let \( p_n \in \mathbb{R}^m \). Let \( p_{n+1} = p_n - \frac{\epsilon}{2} G(q_n)^T \mu \) for \( \mu \in \mathbb{R}^k \). Then,

\[
dq_n \wedge dp_{n+1/2} = dq_n \wedge dp_n
\]

Proof. By direct calculation using eq. (33) from fact 8.

\[
dq_n \wedge dp_{n+1/2} = dq_n \wedge dp_n - dq_n \wedge d\left( \frac{\epsilon}{2} G(q_n)^T \mu \right)
\]

\[
= dq_n \wedge dp_n - \frac{\epsilon}{2} \left( dq_n \wedge d(G(q_n)^T \mu) \right)
\]

\[
= dq_n \wedge dp_n
\]

by fact 22. Fact 22 can be applied since \( g(q_n) = 0 \) and \( \mu \in \mathbb{R}^k \) by assumption.

Corollary 1. For a skew-symmetric matrix \( L \in \text{Skew}(m) \),

\[
dq_n \wedge dp_{n+1/2} + \frac{1}{2} dq_n \wedge L dq_n = dq_n \wedge dp_n + \frac{1}{2} dq_n \wedge L dq_n
\]

Proof. Using lemma 13, add \( \frac{1}{2} dq_n \wedge L dq_n \) to both sides.

Lemma 14. Let \( (q_n, p_{n+1/2}) \in \mathbb{R}^{2m} \). Let \( \Phi : \mathbb{R}^{2m} \to \mathbb{R}^{2m} \) be a symplectic transformation with respect to the magnetic symplectic form \( \Omega_{\text{mag}} \). If \( (q_{n+1}, p_{n+1}) = \Phi(q_n, p_{n+1/2}) \) then,

\[
dq_{n+1} \wedge dp_{n+1} + \frac{1}{2} dq_{n+1} \wedge L dq_{n+1} = dq_n \wedge dp_{n+1/2} + \frac{1}{2} dq_n \wedge L dq_n
\]

Proof. Since \( \Phi \) is symplectic we have,

\[
\Phi^* \Omega_{\text{mag}} = \Omega_{\text{mag}}.
\]

Using eq. (54) from fact 11 we express the symplecteness of \( \Phi \) using coordinate differential one-forms (definition 28):

\[
\Phi^* \Omega_{\text{mag}} = \Omega_{\text{mag}} \implies dq_{n+1} \wedge dp_{n+1} + \frac{1}{2} dq_{n+1} \wedge L dq_{n+1} = dq_n \wedge dp_{n+1/2} + \frac{1}{2} dq_n \wedge L dq_n
\]
The statement of the theorem consists of two parts. That the integrator is symplectic and that the integrator is symmetric. We prove each condition individually.

**Lemma 15.** Let $\mu$ and $\mu'$ be Lagrange multipliers such that eqs. (15) and (17) are satisfied. The integrator in algorithm 3 is symplectic.

**Proof.** At iteration $n$ of the integrator, assume $(q_n, p_n) \in T^*M$. The integrator in algorithm 3 consists of three steps as follows. Let $(q_n, p_n) \in T^*M$.

1. Set $\bar{p}_{n+1/2} = p_n - \frac{\epsilon}{2} G(q_n)^\top \mu$.
2. Compute $(q_{n+1}, \bar{p}_{n+1})$ using algorithm 2 with input $(q_n, \bar{p}_{n+1/2})$, step-size $\epsilon$, and skew-symmetric matrix $L$.
3. Set $p_{n+1} = \bar{p}_{n+1} - \frac{\epsilon}{2} G(q_{n+1})^\top \mu'$.

Notice that $\bar{p}_{n+1/2}, \bar{p}_{n+1} \in \mathbb{R}^m$ but that $(q_{n+1}, p_{n+1}) \in T^*M$ by the choice of Lagrange multipliers $\mu$ and $\mu'$. By eq. (54) from fact 11, the magnetic symplectic 2-form can be written in terms of wedge products as,

$$dq_n \wedge dp_n + \frac{1}{2} dq_n \wedge Ldq_n$$

By fact 14 it suffices to show that the integrator conserves the symplectic 2-form on $T^*M$ under the map $(q_n, p_n) \mapsto (q_{n+1}, p_{n+1})$. Therefore, our proof strategy will be to show that

$$dq_{n+1} \wedge dp_{n+1} + \frac{1}{2} dq_{n+1} \wedge Ldq_{n+1} = dq_n \wedge dp_n + \frac{1}{2} dq_n \wedge Ldq_n$$

Since $g(q_n) = 0$ by assumption (since $q_n \in M$) and $\mu \in \mathbb{R}^k$, we may apply corollary 1 to the first step of the integrator to show that

$$dq_n \wedge dp_{n+1/2} + \frac{1}{2} dq_n \wedge Ldq_n = dq_n \wedge dp_n + \frac{1}{2} dq_n \wedge Ldq_n$$

Applying lemma 13 to $(q_{n+1}, \bar{p}_{n+1})$ in the second step and using the fact that the integrator in algorithm 2 is symplectic by lemma 1 shows that,

$$dq_{n+1} \wedge dp_{n+1} + \frac{1}{2} dq_{n+1} \wedge Ldq_{n+1} = dq_n \wedge dp_{n+1/2} + \frac{1}{2} dq_n \wedge Ldq_n$$

$$= dq_n \wedge dp_n + \frac{1}{2} dq_n \wedge Ldq_n$$

Since $g(q_{n+1}) = 0$ by construction and since $\mu' \in \mathbb{R}^k$, applying corollary 1 a second time to the third step yields

$$dq_{n+1} \wedge dp_{n+1} + \frac{1}{2} dq_{n+1} \wedge Ldq_{n+1} = dq_n \wedge dp_n + \frac{1}{2} dq_n \wedge Ldq_n$$

This verifies that the symplectic structure $\Omega_{can}$ is preserved. Therefore, the integrator is symplectic by fact 14. \qed

**Lemma 16.** Let $\mu$ and $\mu'$ be Lagrange multipliers such that eqs. (15) and (17) are satisfied. Let $\epsilon$ be the integration step-size. Then the integrator in algorithm 3 is symmetric under $\epsilon \mapsto -\epsilon$.

**Proof.** The integrator in algorithm 3 integrator consists of three steps as follows. Let $(q_n, p_n) \in T^*M$.

1. Set $\bar{p}_{n+1/2} = p_n - \frac{\epsilon}{2} G(q_n)^\top \mu$.
2. Compute $(q_{n+1}, \bar{p}_{n+1})$ using algorithm 2 with input $(q_n, \bar{p}_{n+1/2})$, step-size $\epsilon$, and skew-symmetric matrix $L$.
3. Set $p_{n+1} = \bar{p}_{n+1} - \frac{\epsilon}{2} G(q_{n+1})^\top \mu'$.
Notice that \( p_{n+1/2}, p_n \in \mathbb{R}^m \) but that \((q_{n+1}, p_{n+1}) \in T^*M\) by the choice of Lagrange multipliers \( \mu \) and \( \mu' \). To show that the integration scheme is symmetric, consider beginning from position \((q_{n+1}, p_{n+1})\) and applying the three integration steps with a reversed step-size. In the first step, we obtain the update

\[
\bar{p}_{n+1/2} = p_{n+1} + \frac{\epsilon}{2} G(q_{n+1})^\top \mu' 
\]

where the last equality derives from rearranging the defining relation in the third step. Since the integrator in algorithm 2 is symmetric by lemma 1, applying the integrator with step-size \(-\epsilon\) maps \((q_{n+1}, \bar{p}_{n+1})\) to \((q_n, p_{n+1/2})\).

The third integration step with Lagrange multiplier \( \mu \) yields the update,

\[
p_{n+2} = \bar{p}_{n+1/2} + G(q_n)^\top \mu 
\]

By assumption, \((q_n, p_n) \in T^*M\) so that \(g(q_n) = 0\) and \(G(q_n)p_n = 0\). This completes the reversibility argument.

We may now prove theorem 3,

**Proof.** Apply lemmas [15 and 16].

It remains to be discussed the uniqueness of the Lagrange multipliers \( \mu \) and \( \mu' \) appearing in algorithm 3. The following result shows that the Lagrange multipliers are uniquely determined when \( \epsilon \), the integration step-size, is sufficiently small. The following proof technique is taken from Theorem 4.1 in [McLachlan et al., 2012].

**Proposition 1.** Let \( g : \mathbb{R}^m \rightarrow \mathbb{R}^k \) be a constraint function with full-rank Jacobian \( G : \mathbb{R}^m \rightarrow \mathbb{R}^{k \times m} \). Let \((q, p) \in T^*M\). Define,

\[
[(q, p)] \overset{\text{def.}}{=} \{(q, p - G(q)^\top \mu) : \mu \in \mathbb{R}^k\}. 
\]

Let \( \text{Proj}_q : \mathbb{R}^m \times \mathbb{R}^m \rightarrow \mathbb{R}^m \) be defined by \( \text{Proj}_q(q, p) = q \). Let \( \Phi^\epsilon_q \overset{\text{def.}}{=} \text{Proj}_q \circ \Phi^\epsilon_1 \circ \Phi^\epsilon_2 \circ \Phi^\epsilon_1 \) be the projection to the \( q \)-variables of the approximate integrator of magnetic dynamics in Euclidean space from appendix G. Then, for \( \epsilon \) sufficiently small, the equation

\[
g(\Phi^\epsilon_q(q^+, p^+)) = 0 \quad \text{such that} \quad (q^+, p^+) \in [(q, p)]
\]

has a unique solution in a neighborhood of \( \mu = 0 \).

**Proof.** Define the map \( F_\epsilon : \mathbb{R}^k \rightarrow \mathbb{R}^k \) by

\[
F_\epsilon(\mu) = \int_0^1 \frac{\partial}{\partial \epsilon} \left(g(\Phi^\epsilon_q(q, p - G(q)^\top \mu))\right) \bigg|_{\epsilon \tau} \, d\tau. 
\]

If \( \epsilon \neq 0 \) then,

\[
F_\epsilon(\mu) = \frac{g(\Phi^\epsilon_q(q, p - G(q)^\top \mu)) - g(\Phi^\epsilon_0(q, p - G(q)^\top \mu))}{\epsilon} 
\]

\[
= \frac{g(\Phi^\epsilon_q(q, p - G(q)^\top \mu))}{\epsilon}. 
\]

On the other hand if \( \epsilon = 0 \) then,

\[
F_0(\mu) = G(q) \text{Proj}_q \left( \frac{d}{d\epsilon}(\Phi^\epsilon_1 \circ \Phi^\epsilon_2 \circ \Phi^\epsilon_1)(q, p - G(q)^\top \mu) \right) 
\]

\[
= G(q)(p - G(q)^\top \mu) 
\]

\[
= G(q)p - G(q)G(q)^\top \mu. 
\]
since $\Phi_1 \circ \Phi_2 \circ \Phi_1$ has order greater than one. Note that $\nabla_\mu F_0(\mu) = G(q)G(q)^\top$. Thus, if $G(q)$ has full-rank, then $G(q)G(q)^\top$ is invertible and, by the inverse function theorem (fact 2), there is a neighborhood $O$ of $0 \in \mathbb{R}^k$ such that $F_0$ is a diffeomorphism of $O$ and $F_0(O)$. Moreover, since $F_\epsilon$ depends smoothly on $\epsilon$, and since $\epsilon \mapsto \det(\nabla_\mu F_\epsilon)$ is continuous, it follows that for sufficiently small $\epsilon$, there exists a neighborhood $O_\epsilon$ of $0 \in \mathbb{R}^k$ such that $F_\epsilon$ is a diffeomorphism of $O_\epsilon$ and $F_\epsilon(O_\epsilon)$. Moreover, since $F_0(0) = 0$ (since $(q, p) \in T^*M$), we have that $0 \in F_0(O)$. Therefore, for small enough $\epsilon$, it also follows that $0 \in F_\epsilon(O_\epsilon)$.

**Proposition 2.** Let $g : \mathbb{R}^m \to \mathbb{R}^k$ be a constraint function with full-rank Jacobian $G : \mathbb{R}^m \to \mathbb{R}^{k \times m}$, let $q_n, p_n \in \mathbb{R}^m$ with $g(q_n) = 0$. Let $\mu' \in \mathbb{R}^k$ be a Lagrange multiplier chosen such that $G(q_n)[p_n - \frac{\epsilon}{2}G(q_n)^\top \mu'] = 0$. Then $\mu'$ is uniquely defined.

**Proof.** The condition $G(q_n)[p_n - \frac{\epsilon}{2}G(q_n)^\top \mu'] = 0$ can be rearranged as,

$$G(q_n)p_n = \frac{\epsilon}{2}G(q_n)G(q_n)^\top \mu'. \tag{172}$$

Since $\frac{\epsilon}{2}G(q_n)G(q_n)^\top$ is invertible for non-zero $\epsilon$, $\mu'$ is uniquely determined. \qed
I Order of Manifold Integrator

This result requires fact 26, definition 38, and theorem 3.

Theorem 5. The integrator in algorithm 3 has order (see definition 38) at least two.

To prove this result we will first require the following lemma, which was proved in Tripuraneni et al. (2017).

Lemma 17. The single-step subroutine in algorithm 2 has order at least two.

Lemma 18. Let \( \mu \) and \( \mu' \) be constraint-preserving Lagrange multipliers. The integrator in algorithm 3 has order at least one.

Before proving lemma 18, recall that the equations of motion for magnetic Hamiltonian dynamics from eqs. (10) to (12) are

\[
\begin{align*}
\dot{q}_t &= \nabla_p H(q_t, p_t) \\
\dot{p}_t &= -\nabla_q H(q_t, p_t) - \mathbf{L} \nabla_p H(q_t, p_t) - G(q_t) \lambda \\
g(q_t) &= 0.
\end{align*}
\]

The equations of motion may be written in matrix form as,

\[
\begin{pmatrix}
\dot{q}_t \\
\dot{p}_t
\end{pmatrix} = 
\begin{pmatrix}
0 & \text{Id} \\
-\text{Id} & -\mathbf{L}
\end{pmatrix}
\begin{pmatrix}
\nabla_q H(q_t, p_t) \\
\nabla_p H(q_t, p_t)
\end{pmatrix} -
\begin{pmatrix}
0 \\
G(q_t) \lambda
\end{pmatrix}. \tag{176}
\]

Notice that eq. (176) is the first-order term in the Taylor series expansion of the vector field flow in the time variable:

\[
\begin{pmatrix}
q_{t+1} \\
p_{t+1}
\end{pmatrix} = 
\begin{pmatrix}
q_t \\
p_t
\end{pmatrix}
+ \epsilon \begin{pmatrix}
\dot{q}_t \\
\dot{p}_t
\end{pmatrix} + \mathcal{O}(\epsilon^2). \tag{177}
\]

Therefore, our proof strategy will be to establish that the vector field flow and the numerical integrator agree to first order.

**Proof of Lemma 18** Recall further that the manifold integrator in algorithm 3 consists of the following three steps.

1. Set \( \bar{p}_{n+1/2} = p_n - \frac{\epsilon}{2} G(q_n)^\top \mu. \)
2. Compute \((q_{n+1}, \bar{p}_{n+1})\) using algorithm 2 with input \((q_n, \bar{p}_{n+1/2})\), step-size \(\epsilon\), and skew-symmetric matrix \(\mathbf{L}\).
3. Set \( p_{n+1} = \bar{p}_{n+1} - \frac{\epsilon}{2} G(q_{n+1})^\top \mu'. \)

From the fact that algorithm 2 is second order from lemma 17 we have that,

\[
\begin{pmatrix}
q_{n+1} \\
p_{n+1}
\end{pmatrix} = 
\begin{pmatrix}
q_n \\
p_n
\end{pmatrix}
+ \epsilon \begin{pmatrix}
0 & \text{Id} \\
-\text{Id} & -\mathbf{L}
\end{pmatrix}
\begin{pmatrix}
\nabla_q H(q_n, p_{n+1/2}) \\
\nabla_p H(q_n, p_{n+1/2})
\end{pmatrix} + \mathcal{O}(\epsilon^2) \tag{178}
\]

\[
= \begin{pmatrix}
q_n \\
p_n - \frac{\epsilon}{2} G(q_n)^\top \mu
\end{pmatrix} + \epsilon \begin{pmatrix}
0 & \text{Id} \\
-\text{Id} & -\mathbf{L}
\end{pmatrix}
\begin{pmatrix}
\nabla_q H(q_n, p_n) - \frac{\epsilon}{2} G(q_n) \lambda \\
\nabla_p H(q_n, p_n) - \frac{\epsilon}{2} G(q_n)^\top \mu
\end{pmatrix} + \mathcal{O}(\epsilon^2) \tag{179}
\]

\[
= \begin{pmatrix}
q_n \\
p_n + \epsilon \begin{pmatrix}
0 & \text{Id} \\
-\text{Id} & -\mathbf{L}
\end{pmatrix}
\begin{pmatrix}
\nabla_q H(q_n, p_n) \\
\nabla_p H(q_n, p_n)
\end{pmatrix} - \frac{\epsilon}{2} \left( G(q_n)^\top \mu \right)
\end{pmatrix} + \mathcal{O}(\epsilon^2). \tag{180}
\]

Now expanding \( G(q_{n+1}) \) as a Taylor series in \(\epsilon\) shows \( G(q_{n+1}) = G(q_n) + \mathcal{O}(\epsilon) \). Therefore,

\[
p_{n+1} = p_{n+1} - \frac{\epsilon}{2} G(q_{n+1})^\top \mu' \tag{181}
\]

\[
= p_{n+1} - \frac{\epsilon}{2} G(q_n)^\top \mu' + \mathcal{O}(\epsilon^2). \tag{182}
\]

Combining eqs. (180) and (182) yields,

\[
\begin{pmatrix}
q_{n+1} \\
p_{n+1}
\end{pmatrix} = 
\begin{pmatrix}
q_n \\
p_n
\end{pmatrix}
+ \epsilon \begin{pmatrix}
0 & \text{Id} \\
-\text{Id} & -\mathbf{L}
\end{pmatrix}
\begin{pmatrix}
\nabla_q H(q_n, p_n) \\
\nabla_p H(q_n, p_n)
\end{pmatrix} - \epsilon \left( G(q_n)^\top \left( \frac{\mu + \mu'}{2} \right) \right) + \mathcal{O}(\epsilon^2). \tag{183}
\]

Comparing eq. (183) and eq. (176) with \( \lambda = \frac{\mu + \mu'}{2} \) shows that the integrator has order at least one.
Proof of Theorem 5. From lemma 18 we know that the manifold integrator has order at least one. From theorem 3 we know the manifold integrator is symmetric. However, from fact 26 symmetric integrators must have even orders. Therefore, algorithm 3 has order at least two. □
J Proof of Theorem

Theorem. Let $M = \{ q \in \mathbb{R}^m : g(q) = 0 \}$ be a connected manifold such that $G(q)$ has full-rank. Let $T^*M$ be an embedded sub-manifold of $\mathbb{R}^{2m}$ as in definition \[.\] Let $q \in M$ and sample $p \mid q \sim \text{Normal}(0, \text{Id}_m \mid G(q)p = 0)$. Let $H : T^*M \to \mathbb{R}$ be a smooth Hamiltonian of the form in eq. (\[). Let $\hat{\Phi}$ be a symmetric (definition \[\]) and symplectic (definition \[\]) integrator. Consider the transition operator $Q : T^*M \to T^*M$ constructed in algorithm \[. The Markov chain with transition operator $Q$ is stationary for the distribution $\pi(q,p) \propto e^{-H(q,p)}$.

Proof. In this proof, let $z = (q,p)$ and let $H(z) = H(q,p)$. To establish stationarity, it suffices to show that the transition satisfies detailed balance. Let $Z \subset T^*M$ be a region of the cotangent bundle. Suppose that $Z'$ is the image of $Z$ under $Q$ when the positive step-size $\epsilon^*$ is randomly chosen. Suppose further that $Z$ is chosen sufficiently small that the value of the Hamiltonian is constant over $Z$ with value $H(Z)$ and over $Z'$ with value $H(Z')$. By virtue of the fact that the integrator is symplectic, we know $\text{Vol}(Z) = \text{Vol}(Z')$. Let $\delta_\epsilon(z \to z')$ be the indicator function for the condition that $z$ is transformed to $z'$ under $Q$ with the integration step-size $\epsilon$. The probability that a randomly generated $z \sim \pi(z)$ will lie in $Z$, that the positive step-size $\epsilon = +\epsilon^*$ is chosen, and that $z$ will subsequently transition from $Z$ to $Z'$ is,

$$\int_{Z'} \int_Z \frac{\exp(-H(z))}{Z_H} \cdot \frac{1}{2} \cdot \min \left\{ 1, e^{H(z')-H(z)} \right\} \cdot \delta_{+\epsilon^*}(z \to z') \, dz \, dz'$$

(184)

$$= \frac{\exp(-H(Z))}{Z_H} \cdot \text{Vol}(Z) \cdot \frac{1}{2} \cdot \min \left\{ 1, e^{H(Z)-H(Z')} \right\}$$

(185)

$$= \frac{\exp(-H(Z'))}{Z_H} \cdot \text{Vol}(Z') \cdot \frac{1}{2} \cdot \min \left\{ 1, e^{H(Z')-H(Z)} \right\}$$

(186)

$$= \int_Z \int_{Z'} \frac{\exp(-H(z'))}{Z_H} \cdot \frac{1}{2} \cdot \min \left\{ 1, e^{H(z)-H(z')} \right\} \cdot \delta_{-\epsilon^*}(z' \to z) \, dz' \, dz$$

(187)

This last equality is the probability that a randomly generated point $z' \sim \pi(z)$ will lie in $Z'$, that the negative step-size $\epsilon = -\epsilon^*$ is chosen, and that $z'$ will subsequently transition to $Z$. Therefore detailed balance is satisfied, establishing stationarity of $\pi$ for the Markov chain.

Notice that the random selection of the step-size is necessary for this proof to hold. If $\epsilon$ were fixed (say, $\epsilon = +\epsilon^*$) then there could no guarantee that $Z$ overlaps the image of $Z'$ under $Q$ (with the positive step-size). In this case, the probability to transition from $Z'$ to $Z$ would be zero making satisfaction of the detailed balance condition impossible. \qed
K Symplectic Maps Conserve Volume

This result requires definitions 30, 31, 32, 33, and 35 and facts 5 and 7.

For a closer look at the differential geometry, one might ask, “In what sense does conservation of the symplectic structure imply conservation of volume?”

**Theorem 6.** Transformations that preserve the symplectic structure under pullback preserve the Liouville volume form from definition 33.

**Proof.** The Liouville volume form is defined by,
\[
\Lambda \overset{\text{def.}}{=} \frac{(-1)^{m(m-1)/2}}{m!} \Omega \wedge \cdots \wedge \Omega
\]
(188)

If \( \Phi \) is symplectic so that \( \Phi^*\Omega = \Omega \), then using fact 5 immediately implies \( \Phi^*\Lambda = \Lambda \) so that the volume measure is conserved under \( \Phi \).

**Theorem 7.** Let \( \Phi_{mag} \) be the magnetic vector field from from definition 22. Then \( \Phi_{mag} \) preserves the canonical Liouville volume form \( \Lambda_{can} \) from definition 35.

**Proof.** From theorem 6, \( \Phi_{mag} \) conserves the magnetic Liouville volume form
\[
\Lambda_{mag} \overset{\text{def.}}{=} \frac{(-1)^{m(m-1)/2}}{m!} \Omega_{mag} \wedge \cdots \wedge \Omega_{mag}
\]
(189)

Now recall fact 6 which says that the space of volume forms is one-dimensional. Hence any constant (see definition 30), non-vanishing (see definition 31) volume form is proportional to any other constant, non-vanishing volume form. Let \( \Lambda_{can} = c \cdot \Lambda_{mag} \) for some \( c \in \mathbb{R} \) with \( c \neq 0 \). Then,
\[
\Phi^*\Lambda_{can} = \Phi^*(c \cdot \Lambda_{mag})
= c \cdot (\Phi^*\Lambda_{mag})
= c \cdot \Lambda_{mag}
= \Lambda_{can}
\]
(190) (191) (192) (193)

By identification, the determinant from definition 33 is \( \det(\Phi) = 1 \) so that \( \Phi \) also conserves volume with respect to \( \Lambda_{can} \) from fact 7.
L Uniquely Defined Lagrange Multipliers

**Theorem 8.** Let \( M = \{ q \in \mathbb{R}^m : g(q) = 0 \} \) be a connected manifold such that \( G(q) \) has full-rank. Then the Lagrange multipliers \( \lambda \) in the equations of motion

\[
\begin{align*}
\frac{d}{dt}q_i &= \nabla_p H(q_i, p_t) \\
\frac{d}{dt}p_t &= -\nabla_q H(q_t, p_t) - L \nabla_p H(q_t, p) - G(q_t)\top \lambda \\
g(q_t) &= 0
\end{align*}
\]

are uniquely defined.

**Proof.** Write \( g(q) \) in terms of the individual constraint functions by identifying \( g(q) = (g_1(q), \ldots, g_k(q)) \). By definition, \( g(q_t) = 0 \) along a solution of the equations of motion. Therefore,

\[
\frac{d}{dt}g(q_t) = G(q_t) \dot{q}_t = 0.
\]

Differentiating the constraint twice with respect to time yields,

\[
\frac{d^2}{dt^2}g(q_t) = \frac{d}{dt}G(q_t) \dot{q}_t = 0
\]

From Hamilton's equations of motion for constrained motion with a separable Hamiltonian \( H(q, p) = U(q) + \frac{1}{2} p\top p \) we make the identifications:

\[
p_t \overset{\text{def.}}{=} \dot{q}_t
\]

Using the same notation as in [Leimkuhler and Reich, 2005], we define the \( k \)-dimensional vector \( g_{qq}(p_t, p_t) \overset{\text{def.}}{=} [\nabla G(q_t) \cdot p_t] p_t \) whose \( i \)-th component is given by,

\[
(g_{qq}(p_t, p_t))_i \overset{\text{def.}}{=} ([\nabla G(q_t) \cdot p_t] p_t)_i = \sum_{i=1}^k p_t\top (\nabla^2 g_i(q_t))p_t.
\]

Using the fact that \( \ddot{q}_t = -\nabla U(q_t) - L p_t - G(q_t)\top \lambda \) from eq. (195) and \( [\nabla G(q_t) \cdot \dot{q}_t] \dot{q}_t = -G(q_t) \ddot{q}_t \) from eq. (199) we obtain,

\[
\begin{align*}
G(q_t) \left[ -\nabla U(q_t) - L p_t - G(q_t)\top \lambda \right] &= -g_{qq}(p_t, p_t) \\
\implies -G(q_t)G(q_t)\top \lambda &= G(q_t)\nabla U(q_t) + G(q_t)L p_t - g_{qq}(p_t, p_t) \\
\implies \lambda &= -(G(q_t)G(q_t)\top)^{-1} \left[ G(q_t)\nabla U(q_t) + G(q_t)L p - g_{qq}(p_t, p_t) \right].
\end{align*}
\]

The matrix \( G(q_t)G(q_t)\top \) is invertible if \( G(q_t) \) has full-rank and therefore \( \lambda \) will be uniquely defined.
M Strang Splitting

This result requires facts 17 and 18. Let $H(q,p)$ be a smooth Hamiltonian. The purpose of a numerical integrator is to approximate the Hamiltonian vector field flow (definition 10) of $H$ to time $t$, denoted $\Phi(\cdot,t)$.

**Definition 39** (Strang Splitting). Suppose $H(q,p)$ is a Hamiltonian of the form,

$$H(q,p) = H_1(q,p) + \cdots + H_k(q,p)$$

and that the Hamiltonian vector field flow $\Phi_i$ for each $H_i(q,p)$ has a closed-form expression. The technique known as Strang splitting constructs a numerical integrator of $\Phi$ via the composition

$$\hat{\Phi} = \Phi_1 \circ \cdots \circ \Phi_k.$$  \hspace{1cm} (207)

An integrator derived from Strang splitting is a composition of exact solutions to Hamilton’s equations of motion. This fact makes it easy to show that the integrator has certain desirable properties. For instance, they are symplectic.

**Lemma 19.** Strang Splitting Integrators are symplectic.

**Proof.** A composition of Hamiltonian flows is symplectic since each $\Phi_i$ is symplectic from fact 17 and the composition of symplectic transformations forms a group from fact 18. \hfill $\square$

The leapfrog integrator can be derived from a Strang splitting argument. Let $H(q,p) = U(q) + \frac{1}{2} p^\top p$ and let $\Omega_{can}$ be the symplectic structure (with matrix from eq. 5). Let the splitting of $H$ be

$$H(q,p) = \underbrace{1/2 U(q)}_{H_1(q,p)} + \underbrace{1/2 p^\top p}_{H_2(q,p)} + \underbrace{1/2 U(q)}_{H_1(q,p)} .$$

**Lemma 20.** The Hamiltonian vector field flow of $H_1$ to time $t$ is

$$(q_0, p_0 - \frac{t}{2} \nabla U(q_0)) = \Phi_1(q_0, p_0; t).$$

**Proof.** The equations of motion (definition 11) of $H_1$ are

$$\dot{q} = 0$$

$$\dot{p} = -\frac{1}{2} \nabla_q U(q).$$

Noting that $q$ is constant during the motion, the flow of these equations of motion is seen to have a closed-form expression as

$$q_t = q_0 + \int_0^t 0 \, ds = q_0$$

$$p_t = p_0 - \int_0^t \left( \frac{1}{2} \nabla_q U(q_0) \right) \, ds = p_0 - \frac{t}{2} \nabla U(q_0).$$

**Lemma 21.** The Hamiltonian vector field flow of $H_2$ to time $t$ is

$$(q_0 + tp, p_0) = \Phi_2(q_0, p_0; t).$$
Proof. The equations of motion of $H_2$ are
\begin{align}
\dot{q} &= p \\
\dot{p} &= 0
\end{align}
\tag{216, 217}

Noting that $p$ is constant during the motion, the flow of these equations of motion is seen to have a closed-form expression as
\begin{align}
q_t &= q_0 + \int_0^t p_0 \, ds = q_0 + tp_0 \\
p_t &= p_0 - \int_0^t 0 \, ds = p_0.
\end{align}
\tag{218, 219}

**Theorem 9.** The leapfrog integrator is the Strang splitting composition $\Phi_1(\cdot; t) \circ \Phi_2(\cdot; t) \circ \Phi_1(\cdot; t)$.

Proof. Let $(q_0, p_0) \in \mathbb{R}^{2m}$. Recall that the leapfrog integrator to time $t$ is defined as the following series of updates.

1. Compute $p_{t/2} = p_0 - \frac{t}{2} \nabla_q U(q_0)$.
2. Compute $q_t = q_0 + tp_{t/2}$.
3. Compute $p_t = p_{t/2} - \frac{t}{2} \nabla_q U(q_t)$.

Collapsing these updates into a single statement gives:
\begin{align}
q_t &= q_0 + t \left( p_0 - \frac{t}{2} \nabla_q U(q_0) \right) \\
p_t &= p_0 - \frac{t}{2} \nabla_q U(q_0) - \frac{t}{2} \nabla_q U \left( q_0 + t \left( p_0 - \frac{t}{2} \nabla_q U(q_0) \right) \right)
\end{align}
\tag{220, 221}

From lemmas 20 and 21 we have
\begin{align}
\Phi_2(\cdot; t) \circ \Phi_1(\cdot; t)(q_0, p_0) &= \Phi_2 \left( q_0, p_0 - \frac{t}{2} \nabla_q U(q_0) \right) \\
&= \left( q_0 + t \left( p_0 - \frac{t}{2} \nabla_q U(q_0) \right), p_0 - \frac{t}{2} \nabla_q U(q_0) \right).
\end{align}
\tag{222, 223}

Therefore,
\begin{align}
\Phi_1(\cdot; t) \circ \Phi_2(\cdot; t) \circ \Phi_1(\cdot; t)(q_0, p_0) &= \left( q_0 + t \left( p_0 - \frac{t}{2} \nabla_q U(q_0) \right), p_0 - \frac{t}{2} \nabla_q U(q_0) - \frac{t}{2} \nabla_q U \left( q_0 + t \left( p_0 - \frac{t}{2} \nabla_q U(q_0) \right) \right) \right) \\
&= \left( q_0 + t \left( p_0 - \frac{t}{2} \nabla_q U(q_0) \right), p_0 - \frac{t}{2} \nabla_q U(q_0) - \frac{t}{2} \nabla_q U \left( q_0 + t \left( p_0 - \frac{t}{2} \nabla_q U(q_0) \right) \right) \right)
\end{align}
\tag{224}

One sees by inspection that eq. (224) has components equal to eqs. (220) and (221).
N Observations on Magnetic HMC

Specialization to canonical HMC. When using the choice $L = 0_m$, one observes that magnetic manifold HMC reduces to canonical HMC wherein Lagrange multipliers are used to enforce manifold constraints. This is because, when $L = 0_m$, the unconstrained integrator in algorithm 2 reduces to a standard leapfrog step. Note that for the variety of Hamiltonian we have considered, it is not necessary to use an implicitly defined numerical integrator, which was the approach in Brubaker et al. (2012).

Ergodicity of the Markov chain. There exist pathological cases afflicting canonical HMC which cause it to not be ergodic. For instance, for certain choices of step-size and number of steps, the chain may never move from its initial position regardless of the sampled momentum variable. Refer to Bishop (2006), Livingstone et al. (2019) for a discussion. This issue may be averted by combining HMC with a Metropolis-adjusted Langevin diffusion. We note that for $L = 0_m$, a single step of manifold HMC is equivalent (in the $q$-variable) to a discretization of Langevin diffusion. Therefore, one can obtain an ergodic Markov chain by interspersing single steps of canonical HMC into steps of magnetic manifold HMC. Since both procedures satisfy detailed balance with respect to $\pi(q, p)$, the combination of the two will also satisfy detailed balance.