

## Collective Lie–Poisson integrators on $\mathbb{R}^3$

ROBERT I. McLACHLAN

*Institute of Fundamental Sciences, Massey University, Palmerston North, New Zealand*  
r.mclachlan@massey.ac.nz

KLAS MODIN\*

*Department of Mathematical Sciences, Chalmers University of Technology, Gothenburg, Sweden*

\*Corresponding author: klas.modin@chalmers.se

AND

OLIVIER VERDIER

*Department of Mathematics, University of Bergen, Bergen, Norway*  
olivier.verdier@math.uib.no

[Received on 8 July 2013; revised on 8 January 2014]

We develop Lie–Poisson integrators for general Hamiltonian systems on  $\mathbb{R}^3$  equipped with the rigid body bracket. The method uses symplectic realization of  $\mathbb{R}^3$  on  $T^*\mathbb{R}^2$  and application of symplectic Runge–Kutta schemes. As a consequence, we obtain simple symplectic integrators for general Hamiltonian systems on the sphere  $S^2$ .

**Keywords:** Lie–Poisson manifold; Poisson integrator; rigid body bracket; collective Hamiltonian; symplectic Runge–Kutta; Hopf fibration; symplectic realization; Clebsch variables; Cayley–Klein parameters.

### 1. Introduction

The general problem of symplectic integration is the following: given a symplectic manifold  $(M, \omega)$  and a Hamiltonian function  $H \in C^\infty(M)$ , construct a symplectic map that approximates the flow  $\exp(hX_H)$  of the Hamiltonian vector field  $X_H$  on  $M$ . All known symplectic integrators require additional structures, either of the symplectic manifold  $(M, \omega)$  or of the Hamiltonian  $H$ . The main examples are the following.

1. If  $(M, \omega)$  is a symplectic vector space, then symplectic Runge–Kutta methods can be used for arbitrary Hamiltonians (see [Hairer \*et al.\*, 2006](#), Section VI.4 and references therein).
2. If  $M = T^*Q$  with the canonical symplectic form, and  $Q$  is a submanifold of  $\mathbb{R}^n$  characterized by  $Q = \{q \in \mathbb{R}^n \mid c(q) = 0\}$ , then the RATTLE method can be used for (almost) arbitrary Hamiltonians. More generally, RATTLE gives symplectic integrators on symplectic manifolds realized as transverse submanifolds defined by coisotropic constraints (see [McLachlan \*et al.\*, 2013](#) and references therein).
3. If the Hamiltonian function is a sum of explicitly integrable subsystems, then splitting methods give symplectic integrators of arbitrary order (see [McLachlan & Quispel, 2002](#) and references therein).

The first two techniques are based on special types of symplectic manifolds, whereas the last technique is based on a special form of the Hamiltonian function.

Recall that *Poisson structures* are generalizations of symplectic structures. The dual of a Lie algebra is called a *Lie–Poisson manifold*. It has a Poisson structure and is therefore foliated in symplectic leaves (Weinstein, 1983). Such leaves are given by *coadjoint orbits* (Marsden & Ratiu, 1999, Section 14). A *Lie–Poisson integrator* on a Lie–Poisson manifold is a numerical integrator that preserves the Poisson structure and the coadjoint orbits. When restricted to a coadjoint orbit, a Lie–Poisson integrator is thus a symplectic integrator. The RATTLE method can be used to construct Lie–Poisson integrators for general Hamiltonian systems on a Lie–Poisson manifold (Hairer *et al.*, 2006, Section VII.5).

The rigid body bracket (see equation (2.1)) provides  $\mathbb{R}^3$  with the structure of a Lie–Poisson manifold. In this paper we develop Lie–Poisson integrators for general Hamiltonian systems on  $\mathbb{R}^3$ . The coadjoint orbits are spheres, so we also obtain symplectic integrators on  $S^2$ . Compared to the RATTLE approach, our integrators use fewer variables (4 instead of 10) and are less complicated since there are no constraints. A popular integrator for the free rigid body is the *discrete Moser–Veselov algorithm* (Moser & Veselov, 1991) and its higher-order generalizations (Hairer & Vilmart, 2006). Compared to these algorithms, our integrators applied to the free rigid body use fewer variables (4 instead of 8) and are less complicated (especially at high order).

Our construction of Lie–Poisson integrators uses results on *symplectic variables* (also called *Clebsch variables*) and *collective Hamiltonians*, found in work by Marsden & Weinstein (1983), Guillemin & Sternberg (1984) and Libermann & Marle (1987). In particular, we use (Marsden & Weinstein, 1983, Example 3.2) that the momentum map for the action of  $SU(2)$  on  $\mathbb{C}^2$  generalizes the Cayley–Klein parameters for the free rigid body to arbitrary Hamiltonian problems on  $\mathbb{R}^3$  (see also Marsden & Ratiu, 1999, Exercise 15.4-1). Our technique of using symplectic variables can sometimes (but not always) be generalized to other Lie–Poisson manifolds (McLachlan *et al.*, 2014), but in this paper we focus on  $\mathbb{R}^3$ .

The paper is organized as follows. We first give the main result, that symplectic Runge–Kutta methods can be used to construct Lie–Poisson integrators on  $\mathbb{R}^3$ . We then describe the geometry of the problem. Thereafter, we demonstrate the main result; we prove the core part in four different ways. These four proofs reflect the facets of the geometry at hand. We give a numerical example in Section 5 and two plausible applications in Section 6. In Section 7 we give some concluding remarks, pointing to generalizations. Finally, we provide three appendices detailing some computations and coordinate formulae.

## 2. Main result

The cross product provides  $\mathbb{R}^3$  with the structure of a Lie algebra. We identify the dual  $(\mathbb{R}^3)^*$  with  $\mathbb{R}^3$  by the standard inner product. Then the Lie algebra structure on  $\mathbb{R}^3$  induces the *rigid body bracket* (Marsden & Ratiu, 1999, Section 10.1(c)) on  $\mathbb{R}^3$

$$\{F, H\}(\mathbf{w}) := -\mathbf{w} \cdot (\nabla F(\mathbf{w}) \times \nabla H(\mathbf{w})). \quad (2.1)$$

Relative to this Lie–Poisson structure, the Hamiltonian vector field corresponding to a Hamiltonian function  $H \in C^\infty(\mathbb{R}^3)$  is given by

$$X_H(\mathbf{w}) := \mathbf{w} \times \nabla H(\mathbf{w}). \quad (2.2)$$

A map  $\varphi: \mathbb{R}^3 \rightarrow \mathbb{R}^3$  is said to *preserve the Lie–Poisson structure* if

$$\{F \circ \varphi, H \circ \varphi\} = \{F, H\} \circ \varphi \quad \forall F, H \in C^\infty(\mathbb{R}^3). \quad (2.3)$$

Consider the map  $\pi : T^*\mathbb{R}^2 \rightarrow \mathbb{R}^3$  given by

$$\pi : (q_1, q_2, p_1, p_2) \mapsto \frac{1}{4} \begin{pmatrix} 2q_1q_2 + 2p_1p_2 \\ 2q_1p_2 - 2q_2p_1 \\ q_1^2 + p_1^2 - q_2^2 - p_2^2 \end{pmatrix}. \quad (2.4)$$

A Hamiltonian  $H \in C^\infty(\mathbb{R}^3)$  can be lifted to a *collective Hamiltonian*

$$\pi^*H := H \circ \pi \quad (2.5)$$

on the symplectic vector space  $T^*\mathbb{R}^2$ . By construction, the collective Hamiltonian (2.5) is constant on each fibre  $\pi^{-1}(\{w\})$ . The flow of the Hamiltonian vector field  $X_{\pi^*H}$  descends to the flow of  $X_H$ . That is, this diagram commutes:

$$\begin{array}{ccc} T^*\mathbb{R}^2 & \xrightarrow{\exp(X_{\pi^*H})} & T^*\mathbb{R}^2 \\ \downarrow \pi & & \downarrow \pi \\ \mathbb{R}^3 & \xrightarrow{\exp(X_H)} & \mathbb{R}^3 \end{array}$$

This follows from  $X_H(\pi(z)) = T\pi(X_{\pi^*H}(z))$ , which in turn follows from equation (3.2) and  $\pi$  being a Poisson map.

In general, a map  $\Phi : T^*\mathbb{R}^2 \rightarrow T^*\mathbb{R}^2$  descends if there is a map  $\varphi : \mathbb{R}^3 \rightarrow \mathbb{R}^3$  such that this diagram commutes:

$$\begin{array}{ccc} T^*\mathbb{R}^2 & \xrightarrow{\Phi} & T^*\mathbb{R}^2 \\ \downarrow \pi & & \downarrow \pi \\ \mathbb{R}^3 & \xrightarrow{\varphi} & \mathbb{R}^3 \end{array}$$

Note that  $\Phi$  descends if and only if it maps fibres to fibres.

Our strategy for Lie–Poisson integrators on  $\mathbb{R}^3$  is to integrate  $X_{\pi^*H}$  with a symplectic Runge–Kutta method

$$\Phi_h(X_{\pi^*H}) : T^*\mathbb{R}^2 \rightarrow T^*\mathbb{R}^2, \quad (2.6)$$

and then use  $\pi$  to project the result back to  $\mathbb{R}^3$ . To retain the structural properties of the exact flow  $\exp(X_{\pi^*H})$ , the aim is that  $\Phi_h(X_{\pi^*H})$  should descend to a Poisson integrator  $\varphi_h(H) : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ . Our main result is that any symplectic Runge–Kutta method will do.

**THEOREM 2.1** Let  $H \in C^\infty(\mathbb{R}^3)$ , and let  $\pi^*H$ , with  $\pi$  given in equation (2.4), be the corresponding collective Hamiltonian on  $T^*\mathbb{R}^2$ . Then any symplectic Runge–Kutta method  $\Phi_h$  applied to the Hamiltonian vector field  $X_{\pi^*H}$  descends to an integrator  $\varphi_h(H)$  on  $\mathbb{R}^3$  which preserves the Lie–Poisson structure and the coadjoint orbits. The integrator  $\varphi_h(H)$  is consistent with  $X_H$  and has the same order of convergence as  $\Phi_h$ . Moreover,  $\varphi_h$  is equivariant with respect to the rotation group  $\text{SO}(3)$ :

$$\varphi_h(g^*H) = g^{-1} \circ \varphi_h(H) \circ g \quad (2.7)$$

for all  $g(w) := Aw$  with  $A \in \text{SO}(3)$ .

So, in order to get a Lie–Poisson integrator for  $X_H$ , we lift the initial data  $\mathbf{w}_0 \in \mathbb{R}^3$  to any point  $\mathbf{z}_0 \in \pi^{-1}(\{\mathbf{w}_0\})$ , then we integrate with a symplectic Runge–Kutta method  $\Phi_h(X_{\pi^*H})$  to obtain  $\mathbf{z}_{k+1} = \Phi_h(X_{\pi^*H})(\mathbf{z}_k)$ , then we project to get a discrete trajectory  $\mathbf{w}_k := \pi(\mathbf{z}_k)$  in  $\mathbb{R}^3$ . Theorem 2.1 ensures that the map  $\varphi_h(H): \mathbf{w}_k \mapsto \mathbf{w}_{k+1}$  is well defined and is a Lie–Poisson integrator.

REMARK 2.2 The Runge–Kutta method  $\Phi_h$  in Theorem 2.1 requires the vector field  $X_{\pi^*H}$ . An explicit expression for  $X_{\pi^*H}$  is given in Appendix B.

REMARK 2.3 By analogy with the collective Hamiltonian  $\pi^*H$ , we call  $\Phi_h(X_{\pi^*H})$  a *collective integrator*.

The coadjoint orbits are given by 2-spheres in  $\mathbb{R}^3$  with the standard volume form as symplectic form. Thus, the Lie–Poisson integrators in Theorem 2.1 also yield volume-preserving integrators on  $S^2$ .

COROLLARY 2.4 Let  $\tilde{H} \in C^\infty(S^2)$  and let  $\iota: S^2 \hookrightarrow \mathbb{R}^3$  be the natural inclusion. Let  $H \in C^\infty(\mathbb{R}^3)$  be an extension of  $\tilde{H}$ , i.e.,  $\iota^*H = \tilde{H}$ . Then  $\varphi_h(H)$  in Theorem 2.1 induces a volume-preserving integrator  $\tilde{\varphi}_h(\tilde{H})$  for  $X_{\tilde{H}}$  by  $\iota \circ \tilde{\varphi}_h(\tilde{H}) = \varphi_h(H) \circ \iota$ .

### 3. Preliminaries

Before the proofs we recall some facts about Poisson manifolds, group actions and group invariant vector fields. This will make the geometry of the problem more transparent.

#### 3.1 Poisson manifolds

If  $(P_1, \{\cdot, \cdot\}_1)$  and  $(P_2, \{\cdot, \cdot\}_2)$  are two Poisson manifolds (Marsden & Ratiu, 1999, Section 10), then a map  $R: P_1 \rightarrow P_2$  is a *Poisson map* if

$$\{F \circ R, G \circ R\}_1 = \{F, G\}_2 \circ R \quad \forall F, G \in C^\infty(P_2). \quad (3.1)$$

Furthermore, if  $H \in C^\infty(P_2)$  then

$$TR \circ X_{H \circ R} = X_H \circ R. \quad (3.2)$$

See, e.g., Marsden & Ratiu (1999, Proposition 10.3.2).

#### 3.2 Group actions on $\mathbb{C}^2$

Since  $\mathbb{C}^2$  is a complex Hilbert space, it is equipped with a symplectic structure (see, e.g., Marsden & Ratiu, 1999, Section 5.2). Under the vector space isomorphism

$$T^*\mathbb{R}^2 \ni (q_0, q_1, p_0, p_1) \mapsto (q_0 + ip_0, q_1 + ip_1) \in \mathbb{C}^2, \quad (3.3)$$

this symplectic structure is exactly the canonical symplectic structure of  $T^*\mathbb{R}^2$ .

The group  $SU(2)$  of complex special unitary  $2 \times 2$  matrices acts on  $\mathbb{C}^2$  by matrix multiplication. Since this action preserves the Hermitian inner product on  $\mathbb{C}^2$  it is automatically symplectic. Recall that the Lie algebra  $\mathfrak{su}(2)$  of  $SU(2)$  consists of skew Hermitian and trace-free complex matrices. The cross product algebra  $(\mathbb{R}^3, \times)$  can be identified with  $\mathfrak{su}(2)$  by the Lie algebra isomorphism

(Marsden & Ratiu, 1999, Section 9, p. 302)

$$\mathbb{R}^3 \ni (x_1, x_2, x_3) \mapsto \frac{1}{2} \begin{pmatrix} -ix_3 & -ix_1 - x_2 \\ -ix_1 + x_2 & ix_3 \end{pmatrix} \in \mathfrak{su}(2). \quad (3.4)$$

By the isomorphisms (3.3), (3.4), and  $(\mathbb{R}^3)^* \simeq \mathbb{R}^3$ , the projection map (2.4) can be interpreted as a map  $\pi: \mathbb{C}^2 \rightarrow \mathfrak{su}(2)^*$ . If we take this point of view, then  $\pi$  is the *momentum map* associated with the action of  $SU(2)$  on  $\mathbb{C}^2$  (see Appendix A for details). This momentum map is  $SU(2)$ -equivariant, i.e.,  $\pi(A \cdot z) = A \cdot \pi(z)$ , where  $A \in SU(2)$  acts on  $\mathfrak{su}(2)^*$  by the coadjoint action  $\text{Ad}_{A^{-1}}^*: \mathfrak{su}(2)^* \rightarrow \mathfrak{su}(2)^*$  (this action corresponds to the action of  $SO(3)$  on  $\mathbb{R}^3$ ; Marsden & Ratiu, 1999, Proposition 9.2.19). A consequence is that  $\pi$  is a Poisson map (Marsden & Ratiu, 1999, Theorem 12.4.1).

**REMARK 3.1** The map  $\pi$  takes spheres in  $\mathbb{C}^2$  of radius  $r$  into spheres in  $\mathbb{R}^3 \simeq \mathfrak{su}(2)^*$  of radius  $r^2/4$ . That is,

$$\|\pi(z)\|_2 = \frac{1}{4} \|z\|_2^2. \quad (3.5)$$

Much related to  $\pi$  is the map

$$\mathbb{C}^2 \supset S^3 \ni z \mapsto 4\pi(z) \in S^2 \subset \mathbb{R}^3, \quad (3.6)$$

which is a Riemannian submersion. This map yields the classical *Hopf fibration*, i.e., the fibration of  $S^3$  in circles over  $S^2$ .

The Lie group of unitary complex numbers  $U(1)$  acts on  $\mathbb{C}^2$  by

$$(z_1, z_2) \cdot e^{i\theta} = (z_1 e^{i\theta}, z_2 e^{i\theta}). \quad (3.7)$$

We denote this action by  $\Psi_\theta: \mathbb{C}^2 \rightarrow \mathbb{C}^2$ . It preserves each fibre  $\pi^{-1}(\{w\})$ . That is,

$$\pi \circ \Psi_\theta = \pi. \quad (3.8)$$

In fact, the action is transitive in the fibres, so  $U(1)$  gives a parametrization of each fibre. In particular, if  $\Phi$  is  $U(1)$ -equivariant, i.e.,  $\Phi(z \cdot e^{i\theta}) = \Phi(z) \cdot e^{i\theta}$ , then  $\Phi_h$  is descending.

The  $U(1)$  action preserves the Hermitian inner product, so it is symplectic. The orbits are generated by the flow of a Hamiltonian vector field  $X_M$ , with Hamiltonian function

$$M(z_1, z_2) = |z_1|^2 + |z_2|^2. \quad (3.9)$$

Thus,  $M$  is the momentum map for the  $U(1)$  action and may be regarded as a map  $M: \mathbb{C}^2 \rightarrow \mathfrak{u}(1)^* \simeq \mathbb{R}$ .

An illustrative summary of the spaces involved is provided in Fig. 1.

### 3.3 Invariant vector fields

The pullback by a diffeomorphism  $\Psi$  of a vector field  $X$  is defined as

$$\Psi^*X := T\Psi^{-1} \circ X \circ \Psi. \quad (3.10)$$

The following result on arbitrary Runge–Kutta methods is useful.

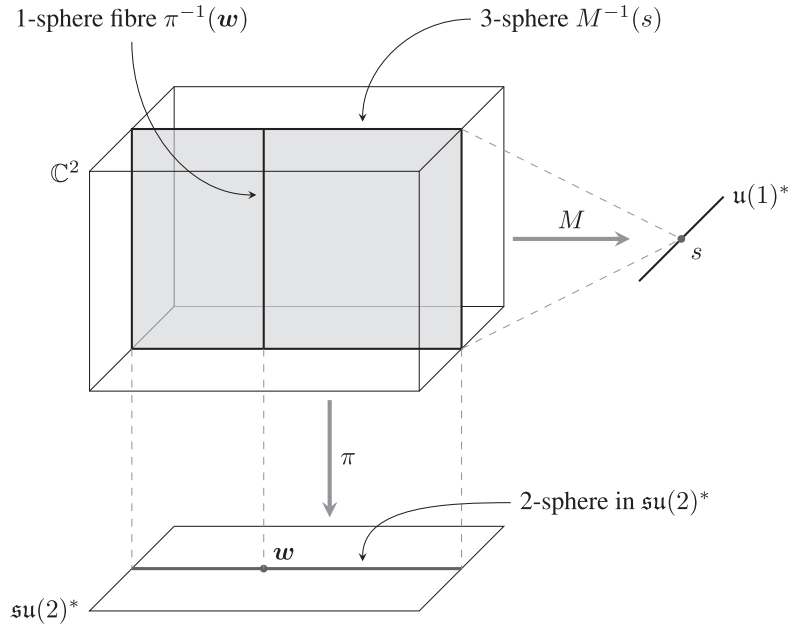


FIG. 1. Visualization of the relation between the spaces involved in the proof. Recall that  $\pi$  is defined by (2.4) and the identification (3.4), and that the momentum map  $M$  is defined by (3.9).

LEMMA 3.2 Let  $G$  be a Lie group which acts linearly on  $\mathbb{C}^n$  by an action map  $\Psi_g$ . Let  $X$  be a  $G$ -invariant vector field on  $\mathbb{C}^n$ , i.e.,

$$\Psi_g^* X = X \quad \forall g \in G. \quad (3.11)$$

Further, let  $\Phi_h(X): \mathbb{C}^n \rightarrow \mathbb{C}^n$  be a Runge–Kutta method applied to  $X$ . Then  $\Phi_h(X)$  is  $G$ -invariant, i.e.,

$$\Psi_g^{-1} \circ \Phi_h(X) \circ \Psi_g = \Phi_h(X) \quad \forall g \in G. \quad (3.12)$$

*Proof.* Runge–Kutta methods are equivariant with respect to affine transformations. Since  $\Psi_g$  is linear this implies

$$\Psi_g^{-1} \circ \Phi_h(X) \circ \Psi_g = \Phi_h(\Psi_g^* X). \quad (3.13)$$

The vector field  $X$  being  $G$ -invariant thus implies

$$\Psi_g^{-1} \circ \Phi_h(X) \circ \Psi_g = \Phi_h(X), \quad (3.14)$$

i.e.,  $\Phi_h(X)$  is  $G$ -invariant.  $\square$

Note that if  $H \in C^\infty(\mathfrak{su}(2)^*)$  then the Hamiltonian vector field  $X_{\pi^* H}$  on  $\mathbb{C}^2$  is  $U(1)$ -invariant. Indeed, the action  $\Psi_\theta$  is symplectic, so equations (3.2) and (3.8) yield

$$\Psi_\theta^* X_{\pi^* H} = X_{\Psi_\theta^* \pi^* H} = X_{\pi^* H}. \quad (3.15)$$

#### 4. Proofs

Theorem 2.1 is proved in three steps:

1. In Section 4.1 we prove, in four different ways, that  $\Phi_h(X_{\pi^*H})$  descends to a Poisson map  $\varphi_h(H)$  which preserves coadjoint orbits.
2. In Section 4.2 we prove that  $\varphi_h(H)$  has the same convergence order as  $\Phi_h(X_{\pi^*H})$ .
3. In Section 4.3 we prove that  $\varphi_h(H)$  is  $SU(2)$ -equivariant.

##### 4.1 Descending property and preservation of coadjoint orbits

**PROPOSITION 4.1** The map  $\Phi_h(X_{\pi^*H}): \mathbb{C}^2 \rightarrow \mathbb{C}^2$  descends to a map  $\varphi_h(H): \mathfrak{su}(2)^* \rightarrow \mathfrak{su}(2)^*$  which preserves the Lie–Poisson structure and the coadjoint orbits.

We give four different proofs of this result. Each proof suggests its own generalization to other Lie–Poisson manifolds. Such generalizations are explored in a forthcoming paper (McLachlan *et al.*, 2014).

To start with, note the special coadjoint orbit at the origin; it has dimension 0, whereas all the others have dimension 2. Furthermore, the fibre above the origin in  $\mathfrak{su}(2)^*$  is the origin in  $\mathbb{C}^2$ , so this *trivial fibre* has dimension 0, whereas all the other fibres have dimension 1. The origin in  $\mathfrak{su}(2)^*$  is an equilibrium point for every Hamiltonian vector field  $X_H$  on  $\mathfrak{su}(2)^*$ , so the origin in  $\mathbb{C}^2$  is an equilibria point for every lifted Hamiltonian vector field  $X_{\pi^*H}$  on  $\mathbb{C}^2$ . Since every Runge–Kutta method exactly preserves equilibria points, the result in Proposition 4.1 is true at the origin. Thus, it remains to prove the result on  $\mathbb{C}^2 \setminus \{0\}$ . Removing the origin simplifies the proofs, since  $\pi: \mathbb{C}^2 \setminus \{0\} \rightarrow \mathfrak{su}(2)^* \setminus \{0\}$  is a submersion, so if  $\Phi: \mathbb{C}^2 \setminus \{0\} \rightarrow \mathbb{C}^2 \setminus \{0\}$  descends to  $\varphi: \mathfrak{su}(2)^* \setminus \{0\} \rightarrow \mathfrak{su}(2)^* \setminus \{0\}$  and  $\Phi$  is smooth, then  $\varphi$  is also smooth (and correspondingly for smooth functions).

The following result is used in the first, second and fourth proofs.

**LEMMA 4.2** Let  $\Phi_h$  be a symplectic Runge–Kutta method on  $\mathbb{C}^2$ . Then the momentum map  $M$  in equation (3.9) is conserved by  $\Phi_h(X_{\pi^*H})$ .

*Proof.* The momentum  $M$  associated with the  $U(1)$  action is quadratic. Since  $M$  is an invariant of  $X_{\pi^*H}$ , and since symplectic Runge–Kutta methods conserve quadratic invariants (Hairer *et al.*, 2006, Theorem VI.7.6), we get that  $\Phi_h(X_{\pi^*H})$  conserves  $M$ .  $\square$

The following result is used in the first and fourth proofs.

**LEMMA 4.3** Let  $\Phi: \mathbb{C}^2 \rightarrow \mathbb{C}^2$  be a map that descends and conserves the momentum map  $M$  in equation (3.9). Then the descending map  $\varphi: \mathfrak{su}(2)^* \rightarrow \mathfrak{su}(2)^*$  preserves the coadjoint orbits.

*Proof.* The action of  $SU(2)$  on  $\mathbb{C}^2$  is norm preserving. For every  $A \in SU(2)$ ,  $z$  and  $A \cdot z$  belong to the same level set of  $M$  because  $M(z) = \|z\|^2$ .

Let  $z' := \varphi(z)$ . Then  $z$  and  $z'$  belong to the same level set of  $M$ . Since  $SU(2)$  acts transitively on that level set (Marsden & Ratiu, 1999, Equation (9.2.15)), there is an  $A \in SU(2)$  such that  $z' = A \cdot z$ . By equivariance of the momentum map  $\pi$ , we conclude that  $\pi(z') = A \cdot \pi(z)$ , so the descending map  $\varphi$  preserves the coadjoint orbit.  $\square$

**4.1.1 Symmetry + conservation of momentum.** The first proof we consider is based on two key properties: (i) the Hamiltonian  $\pi^*H$  is invariant with respect to the  $U(1)$  action and (ii) symplectic Runge–Kutta methods conserve the momentum  $M$  associated with the  $U(1)$  action.

*First proof of Proposition 4.1.* We observed in equation (3.15) that  $X_{\pi^*H}$  is  $U(1)$ -equivariant. It therefore follows from Lemma 3.2 that  $\Phi_h(X_{\pi^*H})$  is  $U(1)$ -equivariant. The  $U(1)$  action parametrizes the fibres, so  $\Phi_h(X_{\pi^*H})$  descends to a map  $\varphi_h(H)$ . It preserves the Lie–Poisson structure, since  $\Phi_h(X_{\pi^*H})$  is symplectic and  $\pi$  is a Poisson map.

Finally, we conclude that  $\varphi_h(H)$  preserves the coadjoint orbits by appealing to Lemmas 4.2 and 4.3.  $\square$

**4.1.2 Backward error analysis + conservation of momentum.** The idea in this proof is to use *backward error analysis* of numerical integrators. More precisely, we follow the framework developed in Hairer *et al.* (2006, Section IX). Throughout this section and the next, a truncated modified Hamiltonian for the symplectic Runge–Kutta method  $\Phi_h(X_{\pi^*H})$  is denoted by  $F_h$  (i.e., an arbitrary truncation of the series in Hairer *et al.*, 2006, Equation (IX.3.4)).

*Second proof of Proposition 4.1.* In terms of backward error analysis, Lemma 4.2 states that

$$\langle dM, X_{F_h} \rangle = 0. \quad (4.1)$$

We now have

$$0 = \langle dM, X_{F_h} \rangle = \{M, F_h\} = -\{F_h, M\} = -\langle dF_h, X_M \rangle. \quad (4.2)$$

Since  $X_M$  generates the  $U(1)$  orbits, and since the  $U(1)$  orbits parametrize the fibres, the equality  $\langle dF_h, X_M \rangle = 0$  implies that  $F_h$  is constant on the fibres. Thus,  $F_h = \pi^*\tilde{H}_h$  for some function  $\tilde{H}_h$  on  $\mathfrak{su}(2)^*$ . When restricted to  $\mathfrak{su}(2)^* \setminus \{0\}$  this function is smooth. Therefore, by equation (3.2), the Hamiltonian vector field  $X_{F_h}$  restricted to  $\mathbb{C} \setminus \{0\}$  descends to the Hamiltonian vector field  $X_{\tilde{H}_h}$  on  $\mathfrak{su}(2)^* \setminus \{0\}$ , which implies that the flow  $\exp(hX_{F_h})$  descends to  $\exp(hX_{\tilde{H}_h})$ . Since this is true for all truncations of modified Hamiltonians  $F_h$ , it follows from Hairer *et al.* (2006, Theorem IX.5.2) that  $\Phi_h(X_{\pi^*H})$  descends to a Poisson map that preserves coadjoint orbits.  $\square$

**4.1.3 Backward error analysis + trivial cohomology.** In this proof we again use backward error analysis, but instead of conservation of momentum we use equivariance of Runge–Kutta methods and that a certain cohomology class is trivial. The notation is the same as in the previous proof.

*Third proof of Proposition 4.1.* To conduct backward error analysis we examine the group of  $U(1)$ -equivariant diffeomorphisms and its formal Lie algebra. The set of all  $U(1)$ -equivariant diffeomorphisms on  $\mathbb{C}^2$  forms a group denoted by  $\text{Diff}_{U(1)}(\mathbb{C}^2)$ . The corresponding algebra is given by the space of  $U(1)$ -invariant vector fields and is denoted by  $\mathfrak{X}_{U(1)}(\mathbb{C}^2)$ . Since  $X_M$  generates the  $U(1)$  orbits, it follows that

$$X \in \mathfrak{X}_{U(1)}(\mathbb{C}^2) \iff [X, X_M] = 0. \quad (4.3)$$

We have already seen in equation (3.15) that  $X_{\pi^*H} \in \mathfrak{X}_{U(1)}(\mathbb{C}^2)$ . Since Runge–Kutta methods are equivariant with respect to affine transformations, and since the  $U(1)$  action is linear, Lemma 3.2 gives

that  $\Phi_h(X_{\pi^*H}) \in \text{Diff}_{U(1)}(\mathbb{C}^2)$ . In terms of backward error analysis, this means that  $X_{F_h} \in \mathfrak{X}_{U(1)}(\mathbb{C}^2)$ , i.e.,

$$[X_{F_h}, X_M] = 0. \quad (4.4)$$

We now get

$$X_{\{M, F_h\}} = [X_{F_h}, X_M] = 0, \quad (4.5)$$

which implies that  $\{M, F_h\}$  is constant, so  $\langle dF_h, X_M \rangle = c$  for some constant  $c \in \mathbb{R}$ .

In order to show that  $c = 0$ , we consider one fixed  $U(1)$ -orbit  $O$ , for instance, the one passing through  $z_0 = (1, 0)$ . Let  $\iota: O \hookrightarrow \mathbb{C}^2$  be the inclusion of  $O$  into  $\mathbb{C}^2$ . Since  $O$  is a closed manifold we get

$$\begin{aligned} 0 &= \int_O d\iota^* F_h \\ &= \int_O d(F_h(\Psi_\theta(z_0))) \\ &= \int_0^{2\pi} \left\langle dF_h(\Psi_\theta(z_0)), \frac{d\Psi_\theta(z_0)}{d\theta} \right\rangle d\theta \\ &= \int_0^{2\pi} \underbrace{\langle dF_h(\Psi_\theta(z_0)), X_M(\Psi_\theta(z_0)) \rangle}_c d\theta \\ &= c \int_0^{2\pi} d\theta = 2\pi c, \end{aligned} \quad (4.6)$$

which implies  $c = 0$ . Thus,  $\langle dF_h, X_M \rangle = 0$ , so  $F_h$  is constant on the fibres. Repeating the last part of the previous proof,  $\Phi_h(X_{\pi^*H})$  descends to a Poisson map which preserves coadjoint orbits.  $\square$

The last part of the proof hinges on a property of the fibration related to the cohomology of the corresponding quotient space. The property is that if a one-form is a pullback by  $\pi$  and is closed, then it is the exterior differential of a function which is also a pullback by  $\pi$ . The meaning of equation (4.6) is to show that this holds, in other words, that the cohomology associated to the fibration is trivial.

**REMARK 4.4** Concerning the cohomology above, we believe there is a minor mistake in [Hairer et al. \(2006, Theorem IX.5.7\)](#). The theorem states that any left invariant symplectic integrator on the cotangent bundle  $T^*G$  of a Lie group  $G$  descends to a Poisson integrator on  $\mathfrak{g}^*$  which preserves coadjoint orbits. The statement that coadjoint orbits are preserved is true only if the cohomology class of  $G$ -invariant one-forms on  $G$  is trivial. This is not always the case, not even locally.

**4.1.4 Collective approach.** We use that  $SU(2)$  acts symplectically on  $\mathbb{C}^2$  and that the Hopf map is the equivariant momentum map for the action. This proof does not use backward error analysis.

*Fourth proof of Proposition 4.1.* We know from Lemma 4.2 that  $M$  is preserved. Since  $\Phi_h$  is symplectic, it preserves the symplectic orthogonal directions. Indeed, suppose that  $X$  and  $Y$  are two symplectically orthogonal vectors, i.e.,  $\omega(X, Y) = 0$ . By symplecticity of  $\Phi_h$  we have

$$\omega(T\Phi_h X, T\Phi_h Y) = \omega(X, Y) = 0, \quad (4.7)$$

so  $T\Phi_h(X)$  and  $T\Phi_h(Y)$  are symplectic orthogonal.

The symplectic orthogonal direction to a tangent space of a level set of  $M$  is the fibre direction at that point, since any tangent vector  $X$  of a level set of  $M$  fulfils  $\omega(X_M, X) = \langle dM, X \rangle = 0$ . If  $z \in \mathbb{C} \setminus \{0\}$  then, by a dimension argument,  $X_M(z) \neq 0$  is the only direction that is symplectic orthogonal to the tangent space at  $z$  of the level sets of  $M$ .

Take two points  $z, z'$  in a nontrivial fibre. There is a curve in that fibre which joins these two points. The image of that curve by  $\Phi_h$  is another curve, which is tangent at all its points to the fibre direction. As a result, that image curve also lies in a fibre. Its end points  $\Phi_h(z)$  and  $\Phi_h(z')$  are thus in the same fibre, from which we conclude that  $\Phi_h$  is fibre preserving.

Finally, we conclude that the descending method  $\varphi_h$  preserves the coadjoint orbits by appealing to Lemmas 4.2 and 4.3.  $\square$

#### 4.2 Convergence order

PROPOSITION 4.5 Let  $\Phi_h(X_{\pi^*H})$  be an integrator of order  $k$  for  $X_{\pi^*H}$  that descends to  $\varphi_h(H)$ . Then  $\varphi_h(H)$  is an integrator of order  $k$  for  $X_H$ .

*Proof.* We have

$$\Phi_h(X_{\pi^*H})(z) = \exp(hX_{\pi^*H})(z) + \mathcal{O}(h^{k+1}). \quad (4.8)$$

Since  $\pi$  is smooth this yields

$$(\pi \circ \Phi_h(X_{\pi^*H}))(z) = (\pi \circ \exp(hX_{\pi^*H}))(z) + \mathcal{O}(h^{k+1}). \quad (4.9)$$

Next, since  $\Phi_h(X_{\pi^*H})$  and  $\exp(hX_{\pi^*H})$  descend we get

$$\varphi_h(H)(\pi(z)) = \exp(X_H)(\pi(z)) + \mathcal{O}(h^{k+1}). \quad (4.10)$$

The result now follows since  $\pi$  is surjective.  $\square$

#### 4.3 Equivariance

Let  $\Psi_A, \psi_A$  denote the action of  $A \in \mathrm{SU}(2)$  on  $\mathbb{C}^2, \mathfrak{su}(2)^*$ , respectively (see Section 3.2).

PROPOSITION 4.6 Assume that  $\Phi_h(X_{\pi^*H})$  descends to  $\varphi_h(H)$ . Further, assume that  $\Phi_h$  is  $\mathrm{SU}(2)$ -equivariant, i.e.,

$$\Phi_h(\Psi_A^* X) = \Psi_A^{-1} \circ \Phi_h(X) \circ \Psi_A \quad (4.11)$$

for all vector fields  $X$  on  $\mathbb{C}^2$ . Then  $\varphi_h(H)$  is also  $\mathrm{SU}(2)$ -equivariant, i.e.,

$$\varphi_h(\psi_A^* H) = \psi_A^{-1} \circ \varphi_h(H) \circ \psi_A. \quad (4.12)$$

*Proof.* From equation (3.2) we get  $X_{\Psi_A^* H} = \Psi_A^* X_H$ , because  $\Psi_A$  is a Poisson map. By  $\mathrm{SU}(2)$ -equivariance of  $\pi$  one has  $\pi \circ \Psi_A = \psi_A \circ \pi$ . Therefore,

$$\Phi_h(X_{\pi^* \psi_A^* H}) = \Phi_h(X_{\Psi_A^* \pi^* H}) \quad \text{by equivariance of } \pi \quad (4.13)$$

$$= \Phi_h(\Psi_A^* X_{\pi^* H}) \quad \text{because } \Psi_A \text{ is Poisson} \quad (4.14)$$

$$= \Psi_A^{-1} \circ \Phi_h(X_{\pi^* H}) \circ \Psi_A \quad \text{by equivariance of } \Phi_h. \quad (4.15)$$

Now  $\varphi_h(H)$  is defined by  $\varphi_h(H) \circ \pi = \pi \circ \Phi_h(X_H)$  so we have

$$\varphi_h(\psi_A^* H) \circ \pi = \pi \circ \Phi_h(X_{\pi^* \psi_A^* H}) \quad (4.16)$$

$$= \pi \circ \Psi_A^{-1} \circ \Phi_h(X_H) \circ \Psi_A \quad (4.17)$$

$$= \psi_A^{-1} \circ (\pi \circ \Phi_h(X_H)) \circ \Psi_A \quad (4.18)$$

$$= \psi_A^{-1} \circ \varphi_h(H) \circ \pi \circ \Psi_A \quad (4.19)$$

$$= \psi_A^{-1} \circ \varphi_h(H) \circ \psi_A \circ \pi. \quad (4.20)$$

We conclude that  $\varphi_h(\psi_A^* H) = \psi_A^{-1} \circ \varphi_h(H) \circ \psi_A$  because  $\pi$  is surjective.  $\square$

## 5. Numerical example

The free rigid body is a standard test problem for Lie–Poisson integrators on  $\mathbb{R}^3$  (Hairer *et al.*, 2006, Section VII.5). The Hamiltonian is

$$H(w_1, w_2, w_3) = \frac{1}{2} \sum_{i=1}^3 \frac{w_i^2}{I_i}, \quad (5.1)$$

for given moments of inertia  $I_1, I_2$  and  $I_3$ .

This problem is integrated with the collective integrator  $\Phi_h(X_{\pi^* H})$ , using the implicit midpoint rule as symplectic Runge–Kutta method. We chose various initial data lifted to fibres above the sphere of radius 1. The resulting trajectories, projected back to  $\mathbb{R}^3$ , are plotted in Fig. 2(a). The energy evolution is plotted in Fig. 2(b) (short-time) and in Fig. 2(c) (long-time).

## 6. Application outlook

As pointed out in Corollary 2.4, a significant feature of the collective integrators described in this paper is that they can be used for *general* Hamiltonian systems on  $S^2$ . In this section we propose two potential applications, both concerned with global atmospheric dynamics. These applications will be developed in detail in future work.

### 6.1 Particle tracking for incompressible flows on $S^2$

The outcome of a global weather simulation is often a time-dependent divergence-free vector field on  $S^2$  describing the infinitesimal evolution of fronts. If a smooth enough, e.g.,  $C^1$ , interpolation of the computed vector field is known, then the collective integrator in Theorem 2.1 can be used to accurately track the flow of individual particles, while exactly conserving mass (since the computed flow is volume preserving).

### 6.2 Point vortex dynamics

The study of point vortices on two-dimensional manifolds is a ‘classical mathematics playground’ according to Aref (2007). More than a playground, point vortices on the sphere provide models for various phenomena in global geophysical flows, such as Jupiter’s great red spot, or the Gulf Stream rings in the ocean. Mathematically, the dynamics of  $N$  point vortices on the sphere is described by a

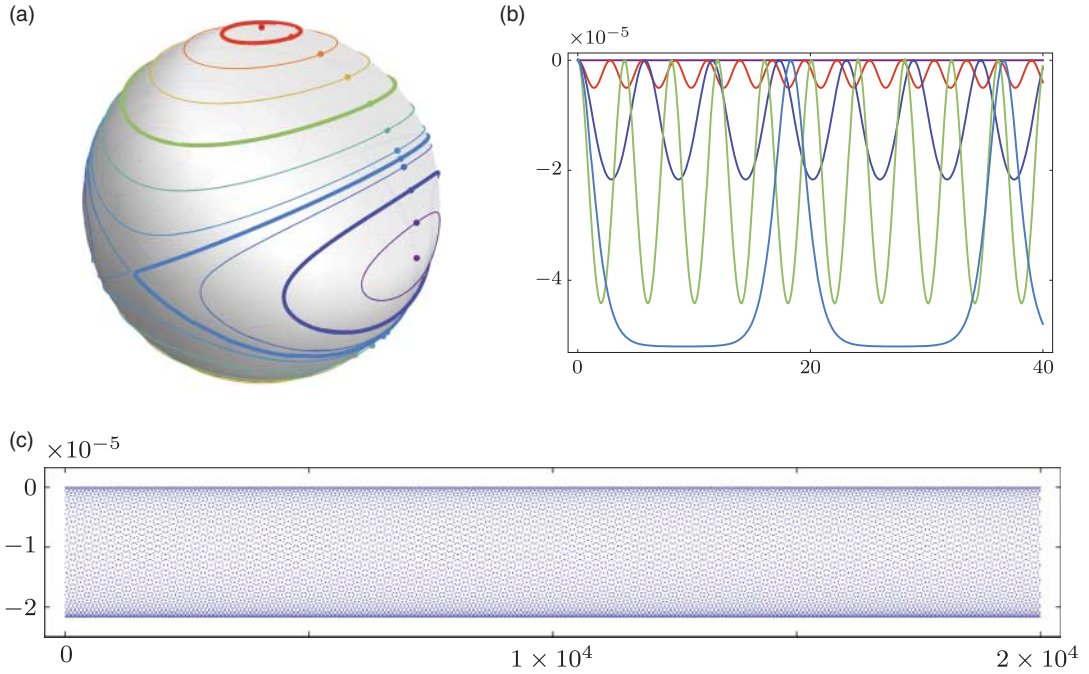


FIG. 2. Simulation of the free rigid body problem with Hamiltonian (5.1). The moments of inertia are  $I_1 = \frac{3}{2}$ ,  $I_2 = 1$  and  $I_3 = \frac{1}{2}$ . We use the midpoint rule as collective integrator. The step size is  $h = 5 \times 10^{-2}$ . (a) Some computed trajectories projected back to  $\mathbb{R}^3$ . Up to machine precision the computed trajectories stay on the sphere, i.e., on a coadjoint orbit. The computed trajectories are qualitatively correct: they are periodic and faithfully capture the dynamics near relative equilibria points. (b) Energy error  $H(w_k) - H(w_0)$  for some computed solutions (corresponding to the thicker trajectories in (a)). The error is larger for trajectories close to the heteroclinic orbits. We observe that the energy is maximal at the initial points. (c) Energy error  $H(w_k) - H(w_0)$  for a long-time simulation ( $4 \times 10^5$  steps). Every 20th step is plotted. There is no drift; the energy error remains bounded.

Hamiltonian system on  $(S^2)^N$  equipped with the product symplectic structure inherited from  $S^2$ . The Hamiltonian is nonseparable so position/momentum-based splitting methods cannot be used. However, by  $N$  copies of the momentum map (2.4), the Hamiltonian on  $(S^2)^N$  can be lifted to a collective Hamiltonian on  $(T^*\mathbb{R}^2)^N \simeq T^*\mathbb{R}^{2N}$ , which can be integrated using a symplectic Runge–Kutta method. From Theorem 2.1 and some bookkeeping related to the product symplectic structure, it follows that the method will descend to a symplectic integrator on  $(S^2)^N$ .

## 7. Conclusion

The present study exploits the geometry of the extended Hopf map in detail. It is natural to ask for which symplectic manifolds other than  $S^2$ , and for which Lie–Poisson manifolds other than  $\mathfrak{su}(2)^*$ , can similar ideas be developed. We address this in McLachlan *et al.* (2014). The starting point in all cases is a symplectic realization  $\pi : M \rightarrow P$  of the Poisson manifold  $P$  by a symplectic vector space  $M$ , associated with a linear symplectic action on  $M$ . The momentum map  $\pi$  is then necessarily quadratic and is conserved by the collective midpoint rule on  $M$ , as in the present study. Thus, in principle, the leaves of  $P$  can be much more complicated than  $S^2$ . However, the space of *all* linear symplectic actions is much too complicated to be treated in general, encompassing a good part of representation theory and

singular Hamiltonian reduction; the details of the geometry of specific maps  $\pi$  need to be taken into account. In [McLachlan \*et al.\* \(2014\)](#) we develop this point of view and construct collective symplectic integrators, based on symplectic Runge–Kutta methods, for various classical cases including  $\mathfrak{sp}(2n, \mathbb{R})^*$ ,  $\mathfrak{so}(n)^*$  and  $\mathfrak{u}(n)^*$ .

## Funding

The research was supported by the Spade Ace Project and the J C Kempe Memorial Fund, the Swedish Research Council (contract VR-350-2012-335), and the Marsden Fund of the Royal Society of New Zealand.

## REFERENCES

- AREF, H. (2007) Point vortex dynamics: a classical mathematics playground. *J. Math. Phys.*, **48**, 065401.
- GUILLEMIN, V. & STERNBERG, S. (1984) *Symplectic Techniques in Physics*. Cambridge: Cambridge University Press.
- HAIRER, E., LUBICH, C. & WANNER, G. (2006) *Geometric Numerical Integration*. Berlin: Springer.
- HAIRER, E. & VILMART, G. (2006) Preprocessed discrete Moser–Veselov algorithm for the full dynamics of a rigid body. *J. Phys. A*, **39**, 13225–13235.
- LIBERMANN, P. & MARLE, C.-M. (1987) Symplectic geometry and analytical mechanics. *Mathematics and its Applications*, vol. 35. Dordrecht: D. Reidel. Translated from the French by Bertram Eugene Schwarzbach.
- MARSDEN, J. E. & RATIU, T. S. (1999) *Introduction to Mechanics and Symmetry*. New York: Springer.
- MARSDEN, J. & WEINSTEIN, A. (1983) Coadjoint orbits, vortices, and Clebsch variables for incompressible fluids. *Phys. D*, **7**, 305–323.
- McLACHLAN, R. I., MODIN, K., VERDIER, O. & WILKINS, M. (2013) Geometric generalisations of SHAKE and RATTLE. *Found. Comput. Math.*, **14** (2), 339–370.
- McLACHLAN, R. I., MODIN, K. & VERDIER, O. (2014) Collective Integrators, accepted in nonlinearity. Arxiv:1308.6620.
- McLACHLAN, R. I. & QUISP, G. R. W. (2002) Splitting methods. *Acta Numer.*, **11**, 341–434.
- MOSER, J. & VESELOV, A. P. (1991) Discrete versions of some classical integrable systems and factorization of matrix polynomials. *Comm. Math. Phys.*, **139**, 217–243.
- WEINSTEIN, A. (1983) The local structure of Poisson manifolds. *J. Differential Geom.*, **18**, 523–557.

## Appendix A. Computation of the momentum map $\pi$

In this appendix we show, by explicit computations, that the map  $\pi$  in equation (2.4) is the momentum map for the action of  $\mathrm{SU}(2)$  on  $\mathbb{C}^2$ .

First, the infinitesimal generator corresponding to an element  $\xi \in \mathfrak{su}(2)$  is a vector field  $\xi_{\mathbb{C}^2}$  on  $\mathbb{C}^2$  given by

$$\xi_{\mathbb{C}^2}(\mathbf{z}) = \xi \mathbf{z}. \quad (\text{A.1})$$

By the algebra isomorphism (3.4),  $\xi \in \mathfrak{su}(2)$  corresponding to  $(x_1, x_2, x_3) \in \mathbb{R}^3$  is given by

$$\xi = \frac{1}{2} \begin{pmatrix} -ix_3 & -ix_1 - x_2 \\ -ix_1 + x_2 & ix_3 \end{pmatrix}.$$

The pullback of the vector field  $\xi_{\mathbb{C}^2}$  by the symplectic isomorphism (3.3) between  $T^*\mathbb{R}^2$  and  $\mathbb{C}^2$  yields the vector field on  $T^*\mathbb{R}^2$  given by

$$\xi_{T^*\mathbb{R}^2}(q_1, q_2, p_1, p_2) = \frac{1}{2} \begin{pmatrix} p_2 x_1 - q_2 x_2 + p_1 x_3 \\ p_1 x_1 + q_1 x_2 - p_2 x_3 \\ -q_2 x_1 - p_2 x_2 - q_1 x_3 \\ -q_1 x_1 + p_1 x_2 + q_2 x_3 \end{pmatrix}. \quad (\text{A.2})$$

This is a Hamiltonian vector field, corresponding to the Hamiltonian  $I_{x_1, x_2, x_3} \in C^\infty(T^*\mathbb{R}^2)$  given by

$$I_{(x_1, x_2, x_3)}(q_1, q_2, p_1, p_2) = \frac{1}{2}(q_1 q_2 + p_1 p_2)x_1 + \frac{1}{2}(q_1 p_2 - q_2 p_1)x_2 + \frac{1}{4}(q_1^2 + p_1^2 - q_2^2 - p_2^2)x_3. \quad (\text{A.3})$$

By identifying  $(\mathbb{R}^3)^*$  with  $\mathbb{R}^3$ , it follows that the momentum map is given by  $\pi$  in equation (2.4).

## Appendix B. Formulae for $X_{\pi^*H}$

In this appendix we give explicit coordinate formulae for  $X_{\pi^*H}$  expressed in the derivatives of  $H$ . Let  $T_z^*\pi$  denote the *cotangent lift* (Marsden & Ratiu, 1999, Section 6.3) of  $\pi$  at the point  $z = (q_1, q_2, p_1, p_2)$ , i.e., the transpose of the Jacobian matrix of  $\pi$ :

$$T_z^*\pi = \frac{1}{2} \begin{pmatrix} q_2 & p_2 & q_1 \\ q_1 & -p_1 & -q_2 \\ p_2 & -q_2 & p_1 \\ p_1 & q_1 & -p_2 \end{pmatrix}. \quad (\text{B.1})$$

Further, let  $J$  be the canonical symplectic matrix on  $T^*\mathbb{R}^2$ . Then the expression for  $X_{\pi^*H}$  is

$$X_{\pi^*H}(z) = J^{-1} T_z^*\pi \, dH(\pi(z)) = \frac{1}{2} \begin{pmatrix} p_2 & -q_2 & p_1 \\ p_1 & q_1 & -p_2 \\ -q_2 & -p_2 & -q_1 \\ -q_1 & p_1 & q_2 \end{pmatrix} \nabla H(\pi(z)), \quad (\text{B.2})$$

which follows since  $JX_{\pi^*H} = d\pi^*H = \pi^*dH = T^*\pi \circ dH \circ \pi$ .

Note that

$$X_{\pi^*H}(z) = X_{I_{dH(\pi(z))}}(z) = (dH(\pi(z)))_{T^*\mathbb{R}^2}(z), \quad (\text{B.3})$$

i.e., at each point  $z$  the vector field  $X_{\pi^*H}$  is given by the infinitesimal generator corresponding to  $dH(\pi(z)) \in \mathfrak{su}(2)$  evaluated at  $z$ . (This result is called the *Collective Hamiltonian Theorem*; see Marsden & Ratiu, 1999, Theorem 12.4.2.)

## Appendix C. Lifting

One possibility to lift a point from  $\mathbb{R}^3$  to  $T^*\mathbb{R}^2$  is to define a map  $L: (x_1, x_2, x_3) \rightarrow (q_1, q_2, p_1, p_2)$  by  $q_1 = \sqrt{2(\|x\| - x_3)}$ , along with

$$(q_2, p_1, p_2) = (2x_1/q_1, -2x_2/q_1, 0). \quad (\text{C.1})$$

This lifting is singular at the north pole, i.e., when  $x_3 = 1$ . This can be addressed by using the lifting

$$\tilde{L} = \tau \circ L(x_1, -x_2, -x_3), \quad (\text{C.2})$$

and  $\tau(q_1, q_2, p_1, p_2) := (q_2, q_1, p_2, p_1)$ . Note that the lifting is only used once, to lift the initial condition on  $\mathbb{R}^3$  to an initial condition on  $T^*\mathbb{R}^2$ . Recall also Theorem 2.1, which asserts that the choice of the lifting has no influence on the computed values projected to  $\mathbb{R}^3$ .