

THESIS FOR THE DEGREE OF DOCTOR OF PHILOSOPHY

**Geometric discretizations in hydrodynamics:  
from plasma physics to thermal quasi-geostrophy**

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Gothenburg, Sweden 2026

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ISBN 978-91-8103-397-7

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Doktorsavhandlingar vid Chalmers tekniska högskola Ny serie nr 5854

ISSN 0346-718X

DOI: <https://doi.org/10.63959/chalmers.dt/5854>

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Cover: Emergence of large-scale structures in the Hasegawa–Mima model of MHD turbulence (taken from Paper II).

Typeset with L<sup>A</sup>T<sub>E</sub>X

Printed by Chalmers Digitaltryck

Gothenburg, Sweden 2026

# Geometric discretizations in hydrodynamics: from plasma physics to thermal quasi-geostrophy

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## Abstract

Many physical processes are modeled by partial differential equations (PDE), and their efficient discretization is a challenging problem and an active field. A common class of models arising in mathematical physics are PDEs formulated in terms of a Lie–Poisson structure on the dual of infinite-dimensional Lie algebras, such as the Lie algebra of vector fields. They are referred to as *Euler–Arnold systems*. In the present thesis, an important subclass of such equations is addressed, namely equations of incompressible magnetohydrodynamics (MHD) and thermal quasi-geostrophy (TQG) on the sphere. The thesis comprises four papers.

In the first paper, a spatio-temporal discretization of MHD on the sphere is developed. The method fully preserves the underlying Lie–Poisson structure. Space discretization is based on truncation of the Lie–Poisson structure and yields a finite-dimensional Lie–Poisson system. Further, a structure preserving time integrator is developed. This integrator exactly preserves all the Casimirs and nearly preserves the Hamiltonian function in the sense of backward error analysis of symplectic integrators.

In the second paper, the developed structure preserving discretization is applied to Hazeltine’s model of 2D turbulence in magnetized plasma and its two limiting cases, the reduced MHD (RMHD) model and the Charney–Hasegawa–Mima (CHM) model. Simulations reveal the formation of large-scale coherent structures in the long time behavior of some fields, and small scales in other fields, which indicates the presence of both inverse and direct cascades of the conserved quantities.

In the third paper, the global model for thermal quasi-geostrophy (TQG) is developed and its Hamiltonian structure is given. Structure preserving spatio-temporal discretization developed for MHD is adapted for TQG, and the long time behavior is studied.

In the fourth paper, the reduced model of axially symmetric magnetohydrodynamics on the three-sphere is derived and its Hamiltonian formulation is given. The finite dimensional Zeitlin’s matrix model is extended for MHD from 2D to axially symmetric 3D flows of magnetized fluids, yielding the first discrete model for 3D magnetohydrodynamics compatible with the underlying Lie–Poisson structure.

**Keywords:** Magnetohydrodynamics, thermal quasi-geostrophy, geophysical flows, Lie–Poisson structure, magnetic extension, Casimirs, Hamiltonian dynamics, symplectic Runge-Kutta integrators.

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## List of publications

The following papers are included in this thesis:

**Paper I:** K. Modin, **M. Roop**, Spatio-temporal Lie–Poisson discretization for incompressible magnetohydrodynamics on the sphere. *IMA J. Numer. Anal.* Vol. 00, p. 1–36. 2025. <https://doi.org/10.1093/imanum/draf024>

**Paper II:** K. Modin, **M. Roop**, Structure-preserving long-time simulations of turbulence in magnetised ideal fluids. *J. Plasma. Phys.* Vol. 92, E30. 2026. <https://doi.org/10.1017/S002237782610138X>

**Paper III:** **M. Roop**, S. Ephrati, Thermal quasi-geostrophic model on the sphere: Derivation and structure-preserving simulation. *Phys. Fluids.* Vol. 37, 096601. 2025. <https://doi.org/10.1063/5.0281814>

**Paper IV:** **M. Roop**, Hamiltonian formulation and matrix discretization for axisymmetric magnetohydrodynamics. *Preprint.* arXiv:2603.10946. 2026. <https://doi.org/10.48550/arXiv.2603.10946>

Author contribution:

**Paper I:** M.R. developed most of the theoretical framework, contributed to convergence proofs, derived the time integration method, and performed numerical simulations, prepared the draft of the manuscript.

**Paper II:** M.R. implemented the methods in the code `quflow`, performed numerical simulations, formulated and analyzed obtained results, prepared the draft of the manuscript.

**Paper III:** M.R. derived the TQG model, implemented the methods, performed numerical simulations, formulated and analyzed obtained results in collaboration with the coauthor, prepared the draft of the manuscript.

**Paper IV:** Independently developed and written.

## Acknowledgements

First, I would like to thank my supervisors Klas Modin and Robert Berman for continuous support, guidance, and attention to the work. Special thanks to Klas for carefully reading my texts and providing important feedback. I am also grateful to Larisa Beilina for being my examiner and for her help in preparation for the defense. During my time at Chalmers, I have been happy to have excellent heads of unit — Annika Lang (when I started) and Irina Pettersson (when I finished). Thanks for all your help! My thanks also go to David Cohen for making my teaching experience a bit more exciting, and for the feedback on the preliminary version of this thesis.

Further, I would like to thank people, discussions and collaboration with whom have in many ways shaped this thesis and from whom I have learned a great deal. First off, I am grateful to Darryl D. Holm for pointing my attention to the problem that has become central for this thesis, as well as for his hospitality and many inspiring discussions we have had during my visit at Imperial College London. My sincere gratitude goes to Sagy Ephrati, for being an exceptionally good coauthor and always being able to convert my texts into a softer and more readable form. I am thankful to Erik Wahlén for all his support and many interesting discussions we have had together. I also want to thank Tünde Fülöp for always being friendly and kind to me, and for her warm welcome to the "Hotel California". Finally, big thanks to my officemate Gijs Custers for his help with understanding SPDEs, supply with fruits and chocolate (good luck in your chocolate competition with David!), and a ton of fun along the way.

Last but not least, I am enormously grateful to my family.

*Michael Roop*  
*Göteborg, 2026*

# 1 Introduction

Being a professional mathematician, in my work, I have to constantly rely not on proofs, but on feelings, guesses, hypotheses; moving from one fact to another, being driven by the special kind of inspiration that makes one see common features in phenomena that may seem to an outsider absolutely unrelated.

A correct guess goes hand-in-hand with a feeling that further proofs would be completely useless, an almost painful feeling that is unforgettable, but difficult to convey.

---

*V.I. Arnold*

The present thesis is built around two topics: turbulence and geometric numerical integration. Turbulence is a complex phenomenon that is difficult to define rigorously. The famous American physicist Richard Feynman once remarked that "turbulence is the last, great unsolved problem of classical physics". Usually, by turbulent behavior, one means that the velocity and the pressure of a fluid undergo chaotic changes. In other words, if a fluid is set to motion, then sooner or later, the regular (or laminar) flow pattern becomes irregular, involves intricate interactions between the fluid layers. A special place in the theory of turbulence is occupied by magnetohydrodynamic (MHD) turbulence, where the turbulent motions of conducting fluids are accompanied by magnetic field fluctuations. A particular example of a conducting fluid is an ionized gas called a *plasma*. Plasma, recognized as the fourth state of matter, fills 99% of the observable Universe. However, our understanding of the fundamental properties of its dynamics and the mathematical models describing it is still limited.

Magnetohydrodynamical turbulence is closely related to hydrodynamical turbulence in the incompressible Euler equations. The incompressible Euler equations is a fundamental mathematical model to investigate the motion of fluids on different domains (with or without a boundary). Although Euler's equations is the simplest model describing fluids, as it often happens in mathematics, problems with the simplest formulation may remain unsolved for centuries. This is exactly the case of the Euler equations.

The book "Topological Methods in Hydrodynamics" by V. Arnold and B.

Khesin [5] starts with these words: "Hydrodynamics is one of those fundamental areas in mathematics where progress at any moment may be regarded as a standard to measure the real success of mathematical science". The incompressible Euler equations were written as early as in 1757, but the long time behavior of their solutions remains largely unknown. Numerous works have been devoted to understanding the properties of solutions to the Euler equations of hydrodynamics, both by analytical and numerical methods. A fundamental observation was made by V.I. Arnold in the 1960s, who discovered their geodesic nature [3, 5]. Namely, the incompressible Euler equations constitute a geodesic flow on the group of volume preserving diffeomorphisms of the underlying manifold (for instance, the sphere), with respect to the right-invariant  $L_2$  metric. The same formalism has been shown to cover a large variety of equations of mathematical physics. They are referred to as *Euler–Arnold systems*. Among them are inviscid Burger’s equation, barotropic and fully compressible Euler’s equations, magnetohydrodynamics equations, linear and non-linear Schrödinger equations, and many other [27]. Arnold’s discovery gave rise to a new field in mathematics, *geometric fluid mechanics*, that opened up new insights in such fundamental problems as stability criteria for solutions, global existence of solutions, and turbulence of the Earth’s atmosphere.

In the present thesis, we address several examples of Euler–Arnold systems, among them is the system of self-consistent magnetohydrodynamics equations. This model has important applications in astrophysics, physics of plasma, and geophysics [21, 17, 43, 18, 19]. The model describes the motion of conductive incompressible fluids that, on the one hand, transport the magnetic field, and, on the other hand, experience influence from the magnetic field. This leads to an extension of the incompressible Euler model by adding the dynamics of the magnetic field and by including the Lorentz force in the momentum conservation law. Geometrically, the MHD system is a Lie–Poisson flow on the dual of the *magnetic extension* of the Lie algebra of volume preserving diffeomorphisms group.

Resolving the long time behavior of solutions to the Euler equations is a prominent problem in mathematical fluid dynamics and is essential for understanding hydrodynamical turbulence. Many applied questions are directly related to this problem, such as understanding the weather patterns on planets, formation of large scale coherent structures in atmospheric motions. As there is no possibility to create a laboratory for experiments with the atmosphere, the way is to utilize computational facilities. The natural step then is to develop efficient numerical algorithms to simulate the equations of hydrodynamics.

The construction of spatio-temporal discretizations of hydrodynamic equations is a challenging problem, especially when it comes to long time simulations. The interpretation of the Euler equations as geodesic equations on the group of volume preserving diffeomorphisms gave a significant contribution, not only to the development of theoretical tools for studying fluids’ motion, but also paved the way for constructing efficient numerical methods allowing for long time simulations.

Indeed, the Hamiltonian interpretation of Arnold’s observation suggests that the Euler equations constitute a Lie–Poisson flow on the dual of the Lie algebra consisting of divergence-free vector fields. This means that the system admits many (in fact, infinitely many) conservation laws, *Casimirs*. Preservation of Casimirs is vital in long time simulations [1]. Indeed, conservation of Casimirs restricts the set of possible states that can be reached from a given initial state, thus affecting the qualitative long time behavior. Therefore, one should use methods that preserve the underlying Lie–Poisson geometry, and, in particular, Casimirs. And this is where *geometric numerical methods*, another central topic of this thesis, come into play.

The structure preserving discretizations for fluids develop in two steps. First, one needs to discretize the equations in space. The main tool here is the theory of *Berezin–Toeplitz quantization* developed in the works [6, 7, 23, 24, 25]. The main idea is that the infinite-dimensional Poisson algebra of smooth functions is replaced with a finite-dimensional analogue, the Lie algebra of skew-hermitian trace-free matrices with the Lie bracket given by the scaled matrix commutator. This makes it possible to introduce a finite dimensional approximation of the Euler equations — the flow on skew-hermitian matrices known as the Euler–Zeitlin model [49]. Later, Zeitlin extended this approach to incompressible magnetohydrodynamics on the flat torus [50]. One crucial benefit of this approach is that the spatially quantized Euler’s equations constitute a Lie–Poisson flow on  $\mathfrak{su}(N)^*$ , exactly as the continuous equations represent a Lie–Poisson flow on the dual the Lie algebra of divergence-free vector fields.

In the present thesis, we extend this approach to incompressible magnetohydrodynamics, as well as thermal quasi-geostrophy. The resulting quantized MHD system constitutes a finite-dimensional Lie–Poisson flow on the dual of the semidirect product Lie algebra  $\mathfrak{f} = \mathfrak{su}(N) \ltimes \mathfrak{su}(N)^*$ , which is usually referred to as the *magnetic extension* of  $\mathfrak{su}(N)$ , and is a quantized counterpart of the magnetic extension of the Lie algebra of divergence-free vector fields. Analogous results hold for the global TQG model on the sphere.

The second step is to discretize the matrix flow in time in such a way that the quantized analogues of Casimirs are exactly preserved. Such an integrator, the *isospectral symplectic Runge–Kutta method*, has been developed in the works [36, 47] for a large class of *isospectral flows*, including the Euler–Zeitlin model for incompressible Euler’s equations. The main mechanism that allows for constructing such methods is the *discrete Lie–Poisson reduction*.

In the present thesis, we use a similar approach to develop structure preserving Lie–Poisson integrators for Lie–Poisson systems on the dual of the Lie algebra of the form  $\mathfrak{f} = \mathfrak{g} \ltimes \mathfrak{g}^*$ , where  $\mathfrak{g}$  is a  $J$ -quadratic Lie algebra. Such Lie algebras include all the classical Lie algebras. This extends the *isospectral symplectic Runge–Kutta integrators* (IsoSRK) developed by Modin and Viviani [36, 47].

Further, the developed structure preserving discretization is used to investigate

the long time behavior of magnetized fluids and geophysical flows. It is worth mentioning that for the Euler equations there are many results known, in particular those obtained in the works [36, 35, 9]. Namely, the long time behavior of the incompressible Euler equations typically settles on a quasi-periodic motion of 2, 3, or 4 blobs for generic initial conditions. The number of blobs is roughly determined by the value of the total angular momentum normalized by the square root of the enstrophy Casimir, while their motion is closely related to low dimensional integrability of vortex blobs dynamics.

However, much less is known about the long time behavior of MHD. In particular, there are no systematic theoretical and numerical studies of the long time behavior for Hazeltine’s model of MHD turbulence, which generalizes conventional models, such as reduced MHD and the Charney–Hasegawa–Mima (CHM) equation. One may pose the following question: Do formations like those in the ideal hydrodynamics appear also in the various models for reduced magnetized fluids? In the present thesis, we fill in this gap and provide a positive answer to this question. We reveal large scale coherent structures forming in the vorticity field for Hazeltine’s model of turbulence in magnetized fluids. These numerical results indicate the presence of an *inverse kinetic energy cascade*. At the same time, the vorticity evolution of the reduced MHD model is drastically different: it cascades directly and develops small scales with no visible large scale structure along with vast amplification of the magnitude.

A separate part of this thesis addresses the large scale dynamics of a model describing a different type of physics. Namely, we develop the global model of thermal quasi-geostrophy (TQG) on the sphere via subsequent approximations to the thermal rotating shallow water (TRSW) equations. This results in a two-field system of equations describing the dynamics of the potential vorticity and buoyancy (normalized density variation) sharing the same semidirect product Lie–Poisson structure as the reduced MHD equations. This intricate connection through the underlying geometric structures of the two theories (MHD and TQG) based on different physics, makes it possible to adapt the structure preserving discretization developed for MHD to investigate the long time behavior of TQG.

This thesis consists of three introductory chapters followed by research papers. The introductory chapters aim at presenting the necessary theoretical material which could not have been included in the papers and which serves as a complement to the results presented in the papers. We start with a discussion of Hamiltonian and Lie–Poisson systems in Chapter 2 and present the geodesic and Hamiltonian approach to fluids. Further, we give the key methods and approaches for their discretization in Chapter 3. Chapters 2 and 3 are extended versions of those in the author’s Licentiate thesis [41]. We proceed with a discussion of finite-mode truncations for fluids in Chapter 4. We conclude by a summary of the papers included in the thesis.

## 2 Hamiltonian and Lie–Poisson systems

Classical mechanics is one of the first attempts to formulate empirical observations of the macroscopic world in terms of mathematical equations, and goes back to Newton, Lagrange, Euler, and Hamilton. Later, with the development of differential geometry, this classical field got a new breath. Indeed, the modern language of differential geometry formulates classical mechanics in an invariant and coordinate-free way, thus deepening the understanding of underlying fundamental structures and adding to the beauty and elegance of the field. The exposition here mainly follows [4, 5, 30].

### 2.1 Preliminaries from differential geometry

We start with some preliminary notions from Riemannian and symplectic geometry, and Hamiltonian mechanics. As the MHD equations will be the main subject of the present thesis, we shall provide (in a concise manner) background material that will be used to show the Hamiltonian structure of magnetohydrodynamics, which is the main goal of this chapter.

#### 2.1.1 Riemannian structures and connections

Let  $M$  be a real smooth manifold of dimension  $\dim(M) = n$ ,  $C^\infty(M)$  be the space of smooth functions on  $M$ ,  $\mathcal{D}(M)$  be the module of vector fields on  $M$ , and  $\Omega^1(M)$  be the module of differential 1-forms on  $M$ .

**Definition 2.1.** A smooth manifold  $M$  is called *Riemannian*, if it is equipped with a smoothly varying field of scalar products:

$$g_x: T_x M \times T_x M \rightarrow \mathbb{R}, \quad (X, Y) \mapsto g_x(X, Y), \quad x \in M.$$

A smooth manifold  $M$  with a given Riemannian structure  $g$  is denoted by  $(M, g)$ .

The next important construction that we need is a *connection*. The notion of a connection on a smooth manifold  $M$  naturally appears when it comes to the definition of an acceleration in mechanics. Let  $Y \in \mathcal{D}(M)$  be a vector field

on  $M$  that can be thought of as a velocity of a particle, and  $x(t)$  be a path on  $M$ . Then, to find an acceleration of a particle, one needs to compare vectors at different points of the curve  $x(t)$ , which is problematic, since they are elements of different vector spaces. To this end, let us equip the manifold  $M$  with linear isomorphisms  $\lambda(t): T_{x(t)}M \rightarrow T_{x(0)}M$  between the tangent spaces. This way of identification of tangent spaces is called a *connection*. Then, taking images  $Y(t) = \lambda(t)(Y_{x(t)}) \in T_{x(0)}M$  of vectors  $Y(t) \in T_{x(t)}M$ , we get the velocity of variation of the vector field  $Y$  along the path  $x(t)$ :

$$\lim_{t \rightarrow 0} \frac{Y(t) - Y(0)}{t} = \left. \frac{dY(t)}{dt} \right|_{t=0} \in T_{x(0)}M. \quad (2.1)$$

Let  $x(t)$  be the trajectory of another vector field  $X$  on the manifold  $M$ . Then, the derivatives (2.1) at various points of  $M$  give us a vector field  $\nabla_X Y$  on  $M$ , and thus come to the notion of a *covariant derivative*.

**Definition 2.2.** A covariant derivative is a map

$$\nabla_X: \mathcal{D}(M) \rightarrow \mathcal{D}(M), \quad X \in \mathcal{D}(M),$$

that satisfies the conditions

1.  $\nabla_{X_1+X_2} = \nabla_{X_1} + \nabla_{X_2}$
2.  $\nabla_{fX} = f\nabla_X$ ,  $f \in C^\infty(M)$ ,
3.  $\nabla_X(Y_1 + Y_2) = \nabla_X(Y_1) + \nabla_X(Y_2)$
4.  $\nabla_X(fY) = X(f)Y + f\nabla_X(Y)$ ,

where  $X_i, Y_i, X, Y \in \mathcal{D}(M)$ ,  $f \in C^\infty(M)$ .

In other words, the operator  $\nabla$  is  $C^\infty(M)$ -linear with respect to its first argument and is a derivation with respect to the second one. Any connection is determined by its covariant derivative.

The action of the covariant derivative on differential 1-forms is given by the following expression:

$$\langle \nabla_X \alpha, Y \rangle = X \langle \alpha, Y \rangle - \langle \alpha, \nabla_X Y \rangle,$$

where  $\alpha \in \Omega^1(M)$ ,  $X, Y \in \mathcal{D}(M)$ , and brackets  $\langle \cdot, \cdot \rangle$  stand for the natural pairing between 1-forms and vector fields.

By means of the Leibniz rule one can expand the action of the covariant derivative  $\nabla_X$  to tensor fields of higher ranks. In particular, if  $g$  is a metric tensor on a smooth manifold  $M$ , then the action of the covariant derivative  $\nabla_X(g)$  is given by the formula:

$$(\nabla_Z g)(X, Y) = Z(g(X, Y)) - g(\nabla_Z X, Y) - g(X, \nabla_Z Y),$$

where  $X, Y, Z \in \mathcal{D}(M)$ .

For a connection on a tangent bundle one can define a vector field

$$T(X, Y) = \nabla_X Y - \nabla_Y X - [X, Y],$$

where  $X, Y \in \mathcal{D}(M)$ . The map

$$T: \mathcal{D}(M) \times \mathcal{D}(M) \rightarrow \mathcal{D}(M)$$

is called *the torsion tensor* of a given connection.

**Definition 2.3.** A connection on a tangent bundle is called *symmetric*, if its torsion tensor is trivial.

It is well known that there is a unique symmetric connection on a Riemannian manifold, which is also metric, that is  $\nabla_X g = 0$  for any  $X \in \mathcal{D}(M)$ , and it is called *the Levi-Civita connection*.

Further on, for the scalar product  $g(X, Y)$  of vector fields  $X, Y$  in terms of the metric  $g$  we will use the notation  $\langle X, Y \rangle_g$ , as well as  $X \cdot Y$ . For the Lie derivative along some vector field  $X$ , we will use the notation  $L_X$ . The Lie derivative  $L_X$  shows an infinitesimal change of a tensor field along the flow generated by the vector field  $X$ . Also, we will need some properties of the Levi-Civita connection.

**Lemma 2.1.** *Let  $\nabla$  be the Levi-Civita connection, associated with the metric  $g$ , and let  $u, v, w \in \mathcal{D}(M)$ . Then,*

$$\langle w, \nabla(v \cdot u) \rangle_g = \langle \nabla_w v, u \rangle_g + \langle v, \nabla_w u \rangle_g. \quad (2.2)$$

*Proof.* Since  $\nabla$  is the Levi-Civita connection,  $\nabla_w g = 0$ :

$$w(g(v, u)) = g(\nabla_w v, u) + g(v, \nabla_w u) = \langle \nabla_w v, u \rangle_g + \langle v, \nabla_w u \rangle_g.$$

Using the definition of the gradient  $(df)(w) = \langle w, \nabla f \rangle_g$  and putting  $f = g(v, u) = v \cdot u$ , one can write down the left hand side as

$$w(g(v, u)) = (d(v \cdot u))(w) = \langle w, \nabla(v \cdot u) \rangle_g.$$

□

**Corollary 2.1.** *Putting  $w = v$  in (2.2), we get*

$$\langle v, \nabla_v u \rangle_g = \langle v, \nabla(v \cdot u) \rangle_g - \langle \nabla_v v, u \rangle_g. \quad (2.3)$$

**Corollary 2.2.** *Putting  $u = v$  in (2.2), we get*

$$\langle w, \nabla|v|^2 \rangle_g = \langle \nabla_w v, v \rangle_g + \langle v, \nabla_w v \rangle_g \Leftrightarrow \langle v, \nabla_w v \rangle_g = \frac{1}{2} \langle w, \nabla|v|^2 \rangle_g. \quad (2.4)$$

Using the metric  $g$  one can define the *flat operator*,  $\flat: \mathcal{D}(M) \rightarrow \Omega^1(M)$ ,  $X^\flat(\cdot) = g(X, \cdot)$ , and its inverse  $\sharp: \Omega^1(M) \rightarrow \mathcal{D}(M)$ , called *sharp operator*.

**Lemma 2.2.** *Let  $\nabla$  be the Levi-Civita connection, and  $v \in \mathcal{D}(M)$ . Then,*

$$(\nabla_v v)^\flat = L_v v^\flat - \frac{1}{2}d|v|^2.$$

*Proof.* Let  $Y \in \mathcal{D}(M)$  is an arbitrary vector field on  $M$ . We need to prove that

$$J = (\nabla_v v)^\flat(Y) - (L_v v^\flat)(Y) + \frac{1}{2}(d|v|^2)(Y) = 0.$$

Let us use the formula of the action of the Lie derivative on 1-forms:

$$(L_v v^\flat)(Y) = v(v^\flat(Y)) - v^\flat([v, Y]) = v(g(v, Y)) - g(v, [v, Y]).$$

Therefore,

$$J = g(\nabla_v v, Y) - v(g(v, Y)) + g(v, [v, Y]) + \frac{1}{2}(d|v|^2)(Y) \quad (2.5)$$

Taking into account that the torsion of  $\nabla$  is trivial, that is

$$\nabla_v Y - \nabla_Y v = [v, Y],$$

we reduce (2.5) to the form

$$J = g(\nabla_v v, Y) - v(g(v, Y)) + g(v, \nabla_v Y) - g(v, \nabla_Y v) + \frac{1}{2}Y(g(v, v)).$$

Since  $\nabla g = 0$ , then  $v(g(v, Y)) = g(\nabla_v v, Y) + g(v, \nabla_v Y)$ , and

$$J = -g(v, \nabla_Y v) + \frac{1}{2}Y(g(v, v)).$$

Finally, using the property of the Levi-Civita connection (2.4),  $J = 0$ .  $\square$

### 2.1.2 Hamiltonian mechanics

Let  $M$  again be a real smooth manifold of even dimension  $\dim(M) = 2n$ , and let  $\Omega$  be a non-degenerate closed 2-form on  $M$ . Then, the pair  $(M, \Omega)$  is called a *symplectic manifold*.

**Theorem 2.1** (Darboux). *Let  $(M, \Omega)$  be a symplectic manifold. Then, in the neighborhood of  $z \in M$ , there exist local coordinates  $(q_1, \dots, q_n, p_1, \dots, p_n)$ , called *canonical coordinates*, such that*

$$\Omega = \sum_{i=1}^n dp_i \wedge dq_i.$$

This means that all symplectic manifolds locally look similar (there are no local invariants).

**Definition 2.4.** Let  $(M_1, \Omega_1)$  and  $(M_2, \Omega_2)$  be two symplectic manifolds, and let  $\varphi: M_1 \rightarrow M_2$  be a  $C^\infty$ -map. Then  $\varphi$  is called a *symplectic map*, or a *symplectomorphism*, if  $\varphi$  is a diffeomorphism, if  $\varphi^*(\Omega_2) = \Omega_1$ .

**Definition 2.5.** Let  $(M, \Omega)$  be a symplectic manifold. A vector field  $X \in \mathcal{D}(M)$  is called *Hamiltonian*, if there is a function  $H: M \rightarrow \mathbb{R}$ , such that

$$\iota_X \Omega = dH,$$

where  $\iota: \mathcal{D}(M) \times \Omega^k(M) \rightarrow \Omega^{k-1}(M)$  is the contraction of a vector field and a differential form, that is (for  $k = 2$ )  $(\iota_X \Omega)(Y) = \Omega(X, Y)$  for any  $Y \in \mathcal{D}(M)$ .

A Hamiltonian vector field with Hamiltonian  $H$  is denoted by  $X_H$ .

To compute the flow generated by the vector field  $X_H$ , one needs to solve the system

$$\dot{z} = X_H(z),$$

that in canonical coordinates  $(q_1, \dots, q_n, p_1, \dots, p_n)$  can be written as

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial q_i}. \quad (2.6)$$

The equations (2.6) are called *canonical*, or *Hamiltonian*.

**Proposition 2.1.** *Let  $X_H$  be a Hamiltonian vector field with the Hamiltonian  $H$ . Then,*

$$L_{X_H} \Omega = 0.$$

*Proof.* Using the Cartan formula  $L_X = \iota_X \circ d + d \circ \iota_X$ , we get

$$L_{X_H} \Omega = \iota_{X_H} d\Omega + d(\iota_{X_H} \Omega) = d(dH) = 0.$$

□

This property of Hamiltonian vector fields means that Hamiltonian flows are symplectic.

In canonical coordinates, a Hamiltonian vector field can be written as

$$X_H = \sum_{i=1}^n \left( \frac{\partial H}{\partial p_i} \frac{\partial}{\partial q_i} - \frac{\partial H}{\partial q_i} \frac{\partial}{\partial p_i} \right).$$

Let  $F, G$  be two smooth functions on a symplectic manifold  $(M, \Omega)$ . Then, one can define a *Poisson bracket* of functions  $F$  and  $G$  by

$$\{F, G\}(z) = \Omega(X_F(z), X_G(z)), \quad z \in M.$$

**Proposition 2.2.** *Let  $\varphi_t$  be the flow of a Hamiltonian vector field  $X_H$ . Then,*

$$\varphi_t^* \{F, G\} = \{\varphi_t^* F, \varphi_t^* G\} \quad (2.7)$$

for all  $F, G \in C^\infty(M)$ .

Differentiating the expression (2.7) by  $t$  at  $t = 0$ , we get

$$X_H(\{F, G\}) = \{X_H(F), G\} + \{F, X_H(G)\}. \quad (2.8)$$

Further, from the definition of the Poisson bracket, we have

$$\{F, G\} = (\iota_{X_F} \Omega)(X_G) = (dF)(X_G) = X_G(F),$$

which implies that

$$\{\{F, G\}, H\} = X_H(\{F, G\}).$$

Using (2.8), we get

$$\{\{F, G\}, H\} = \{X_H(F), G\} + \{F, X_H(G)\} = \{\{F, H\}, G\} + \{F, \{G, H\}\},$$

which is the Jacobi identity.

**Theorem 2.2.** *The Poisson bracket  $\{\cdot, \cdot\}$  has the following properties:*

- *skew-symmetry*

$$\{F, G\} = -\{G, F\},$$

- *Leibniz rule*

$$\{F, GH\} = \{F, G\}H + G\{F, H\},$$

- *Jacobi identity*

$$\{\{F, G\}, H\} + \{\{G, H\}, F\} + \{\{H, F\}, G\} = 0.$$

*Remark 2.1.* The properties in Theorem 2.2 can serve as a definition of the Poisson bracket. Indeed, a set of smooth functions  $C^\infty(M)$  can be endowed with a bilinear, skew-symmetric operation  $\{\cdot, \cdot\}$  satisfying the Jacobi identity. The pair  $(M, \{\cdot, \cdot\})$  then becomes a *Poisson manifold*.

*Remark 2.2.* A Poisson manifold is a more general object than a symplectic manifold. Indeed, any smooth manifold, not necessarily even-dimensional, can be endowed with a Poisson bracket. At the same time, any symplectic manifold is also a Poisson manifold, where the Poisson structure is induced by the symplectic form.

In canonical coordinates, a Poisson bracket can be written as

$$\{F, H\} = \sum_{i=1}^n \left( \frac{\partial H}{\partial p_i} \frac{\partial F}{\partial q_i} - \frac{\partial H}{\partial q_i} \frac{\partial F}{\partial p_i} \right).$$

Finally, in terms of the Poisson bracket, the canonical equations (2.6) take the form

$$\dot{F} = \{F, H\},$$

where  $F$  is any canonical coordinate function.

Among all Hamiltonian systems, a special place is occupied by *integrable* Hamiltonian systems, i.e., such Hamiltonian systems that can be solved explicitly. The following important theorem gives the integrability conditions for Hamiltonian systems, as well as provides a constructive method of integrating them:

**Theorem 2.3** (Liouville, Arnold). *Let  $H = F_1, F_2, \dots, F_n$  be independent functions on a symplectic manifold  $(M, \Omega)$  in involution, i.e.*

$$\{F_i, F_j\} = 0, \quad i, j = 1, \dots, n,$$

*then the trajectories of the Hamiltonian system (2.6) lie on an invariant  $n$ -dimensional manifold*

$$M_I = \{F_1(p, q) = I_1, \dots, F_n(p, q) = I_n\} \subset (M, \Omega),$$

where  $I_i \in \mathbb{R}$ .

*There exist canonical coordinates  $(I_1, \dots, I_n, \varphi_1, \dots, \varphi_n)$ , such that the symplectic form  $\Omega$  has its canonical form*

$$\Omega = \sum_{i=1}^n dI_i \wedge d\varphi_i,$$

*and Hamilton's equations take their simplest form*

$$\dot{I} = 0, \quad \dot{\varphi} = \omega(I).$$

*If, in addition,  $M_I$  is compact and connected, then it is diffeomorphic to the  $n$ -torus  $T^n$ .*

The canonical coordinates  $(I_1, \dots, I_n, \varphi_1, \dots, \varphi_n)$  are called *action-angle* variables. Note that for Hamiltonian systems it is enough to have only  $n$  independent integrals in involution to find a solution, contrary to general type system of ODEs, for which  $2n$  integrals would be needed.

### 2.1.3 Liouville–Arnold integrability as a particular case of Lie–Bianchi integrability

In the previous section, integrability of Hamiltonian systems was discussed, which culminates in the Liouville–Arnold integrability theorem. However, while the Liouville–Arnold theorem guarantees the existence of action–angle variables, it does not provide a constructive algorithm of finding the angle variables. It turns out that the Liouville–Arnold integrability of Hamiltonian systems can be seen as a particular example of the Lie–Bianchi integrability theorem of general type (systems of) ODEs. Indeed, one may ask the following question: given a system of ODEs, what are the conditions for it to be solved by quadratures? The answer is provided in the framework of the *geometric theory of differential equations* originated from the works of the Norwegian mathematician Sophus Lie. In this section, we briefly discuss its main ideas and show how to construct the angle variables for integrable Hamiltonian systems. Even though it is not used in the thesis directly, it feels important to put the Hamiltonian systems setting in a larger framework of general type ODEs. We refer to the monographs [29, 46] for a more comprehensive discussion.

We start with the simplest case, which is an ODE of the first order:

$$F(t, u, \dot{u}) = 0. \quad (2.9)$$

We observe that the object (2.9) can naturally be thought of as a manifold in the *space of 1-jets*  $J^1 \simeq \mathbb{R}^3(t, u_0, u_1)$ , where the coordinates  $u_0$  and  $u_1$  stand for the unknown function and its derivative:

$$\mathcal{E} = \{F(t, u_0, u_1) = 0\} \subset J^1.$$

The geometric image of a solution to the ODE (2.9) is a curve  $\Gamma^0 = \{u_0 = f(t)\}$ , where  $f(t)$  is a function solving the equation  $F(t, f(t), f'(t)) = 0$ . One can introduce the *first prolongation*  $\Gamma^1 \subset \mathcal{E}$  in the following way:  $\Gamma^1 = \{u_0 = f(t), u_1 = f'(t)\}$ . It is more natural to think of solutions as prolonged curves  $\Gamma^1$ , because  $\Gamma^1$  lies on the equation manifold  $\mathcal{E}$ . However, one would want to have a description of  $\Gamma^1$  in terms of extrinsic objects on the ambient space  $J^1$ .

Let us think of  $\Gamma^1 \subset \mathcal{E}$  as of a trajectory of a certain field of directions on  $\mathcal{E}$ . This field of directions is obtained by intersecting two planes at every point  $\theta$  of  $J^1$ . One of them is naturally the tangent plane  $T_\theta \mathcal{E}$ , and the other one is called the *Cartan plane*. The role of the Cartan plane  $\mathcal{C}_\theta \subset J^1$  is to sort solution curves  $\Gamma^1$  out of all curves on  $\mathcal{E}$ . In terms of the canonical coordinates  $(t, u_0, u_1)$  of  $J^1$ , the *Cartan distribution*  $\mathcal{C}$  is defined as

$$\mathcal{C} = \text{span} \left\langle \frac{\partial}{\partial u_1}, \frac{\partial}{\partial t} + u_1 \frac{\partial}{\partial u_0} \right\rangle.$$

The dual way to define the distribution  $\mathcal{C}$  is as a kernel of the *Cartan 1-form*  $\omega$ :

$$\omega = du_0 - u_1 dt, \quad \mathcal{C} = \ker(\omega).$$



**Definition 2.7.** A transformation  $\Phi: J^k \rightarrow J^k$ ,  $\theta \mapsto \Phi(\theta)$  is called *symmetry*, if  $\Phi^*(\mathcal{C}) = \mathcal{C}$ .

Since the Cartan distribution is defined as a kernel of the Cartan forms, it means that the symmetry transformation  $\Phi_\tau$  (one-parameter group of diffeomorphisms of  $J^k$ ) has to preserve the kernel of Cartan forms:

$$\Phi_\tau^*(\omega_j) = \sum_{\alpha} c_{\alpha}(\tau)\omega_{\alpha}.$$

Let  $X$  be an infinitesimal generator of  $\Phi_\tau$ . Differentiating the above expression with respect to  $\tau$  at  $\tau = 0$ , we get

$$L_X(\omega_j) = \sum_{\alpha} \beta_{\alpha}\omega_{\alpha} \iff L_X(\omega_j) \wedge \omega_0 \wedge \dots \wedge \omega_{k-1} = 0 \quad \text{on } \mathcal{E}, \quad (2.11)$$

which is called the *Lie equation* for the unknown  $X$ .

All symmetries  $X_1, X_2, \dots$  form a Lie algebra  $\text{Sym}(\mathcal{E})$  with respect to a commutator of vector fields. Clearly, any vector field in the Cartan distribution  $X \in \mathcal{C}$  is a symmetry. Such symmetries do not provide new solutions, they move a solution along itself. In other words, Cartan planes are transported along the same solution curve. Such symmetries are called *characteristic* and form an ideal  $\text{Char}(\mathcal{E}) \subset \text{Sym}(\mathcal{E})$ . Taking the quotient  $\mathfrak{sym} = \text{Sym}(\mathcal{E})/\text{Char}(\mathcal{E})$ , one gets the Lie algebra of *shuffle symmetries*.

Let  $c_{ij}^k$  be the structure constants of  $\mathfrak{sym}$ , i.e.  $[X_i, X_j] = \sum_k c_{ij}^k X_k$ . We are now in position to formulate the *Lie–Bianchi integrability theorem* (for a modern proof, we refer to [29, Ch. 1]).

**Theorem 2.4** (Lie–Bianchi). *Let  $\mathfrak{sym} = \langle X_1, X_2, \dots, X_k \rangle$  be a  $k$ -dimensional commutative Lie algebra of shuffle symmetries of the  $k$ -th order ODE  $\mathcal{E}$ , i.e.  $[X_i, X_j] = 0, c_{ij}^k = 0$ . Then,  $\mathcal{E}$  is integrable by quadratures.*

*Remark 2.4.* The condition for the Lie algebra to be commutative can be lifted, and instead we only need solvability of  $\mathfrak{sym}$ . In that case, the integrability algorithm presented below will be different.

The Lie–Bianchi theorem also provides a constructive method of finding the integrals for an integrable ODE  $\mathcal{E}$ .

1. First, we construct a matrix  $A$  as  $A_{ij} = \omega_i^{\mathcal{E}}(X_j)$ , where  $\omega_i^{\mathcal{E}}$  are restrictions of the Cartan forms on the ODE  $\mathcal{E}$ . In what follows, we will omit the superscript standing for the restricted forms and will assume that everything is restricted to  $\mathcal{E}$ .
2. Next, we construct new forms  $\tilde{\omega}_0, \dots, \tilde{\omega}_{k-1}$  as follows:

$$\begin{bmatrix} \tilde{\omega}_0 \\ \vdots \\ \tilde{\omega}_{k-1} \end{bmatrix} = A^{-1} \begin{bmatrix} \omega_0 \\ \vdots \\ \omega_{k-1} \end{bmatrix},$$

and the new forms fulfill  $\tilde{\omega}_i(X_j) = \delta_{ij}$ .

3. In the case of a commutative Lie algebra  $\mathfrak{sym}$ , the new forms  $\tilde{\omega}_i$  are closed, and therefore locally exact, i.e. there exist smooth functions  $H_0, \dots, H_{k-1}$  on  $\mathcal{E}$ , such that  $\tilde{\omega}_i = dH_i$ .
4. The solution curve is found then as an intersection of level sets of the functions  $H_i$ :

$$\Gamma^k = \{H_0 = C_0, \dots, H_{k-1} = C_{k-1}\} \subset \mathcal{E}.$$

The constants  $C_0, \dots, C_{k-1}$  are usually referred to as *integration constants*.

Let us make a connection to the integrability of Hamiltonian systems. A Hamiltonian flow is a flow on a symplectic manifold  $(M, \Omega)$  with local coordinates  $(q_1, \dots, q_n, p_1, \dots, p_n)$ . Suppose that we know  $n$  independent commuting integrals  $H = H_1, \dots, H_n \in C^\infty(M)$ , such that  $\{H_i, H_j\} = 0$ . The corresponding Hamiltonian vector fields  $X_{H_1}, \dots, X_{H_n}$  also commute, i.e.  $[X_{H_i}, X_{H_j}] = 0$ . Let  $L^c$  be the invariant Lagrangian manifold given by the level sets of Hamiltonians:

$$L^c = \{H_1 = c_1, \dots, H_n = c_n\} \subset M.$$

The vector fields  $X_{H_1}, \dots, X_{H_n}$  are independent, because  $H_1, \dots, H_n$  are independent. Therefore  $\{X_{H_i}\}$  form a basis on  $L^c$ . We observe that the set of vector fields  $X_{H_2}, \dots, X_{H_n}$  are symmetries of the Hamiltonian flow on  $L^c$  generated by the vector field  $X_H = X_{H_1}$ , due to the vanishing commutators  $[X_{H_i}, X_{H_j}] = 0$ , and  $X_{H_2}, \dots, X_{H_n}$  are transversal to  $X_H$ . This means that the Hamiltonian flow has a commutative Lie algebra of shuffle symmetries of dimension  $n - 1$ . Thus we find ourselves exactly in the framework of the Lie–Bianchi integrability theorem, which implies the existence the 1-forms  $\omega_2^c, \dots, \omega_n^c$ , originating from the Cartan forms for equations (2.6), such that  $\omega_i^c(X_{H_j}) = \delta_{ij}$ , and therefore the forms  $\omega_2^c, \dots, \omega_n^c$  are locally exact, i.e.  $\omega_i^c = d\varphi_i^c$ ,  $i = 2, \dots, n$ , for some functions  $\varphi_i^c$  on  $L^c$ . Finally, according to the Lie–Bianchi theorem, solution to the corresponding Hamiltonian system is given by

$$H_1 = c_1, \dots, H_n = c_n, \quad \varphi_2 = C_2, \dots, \varphi_n = C_n. \quad (2.12)$$

Indeed,  $2n - 1$  constraints (2.12) on the  $2n$ -dimensional manifold  $M$  define the trajectory of the vector field  $X_H$ .

## 2.2 Lie–Poisson systems

One of the most fundamental examples of a Poisson structure is the *Lie–Poisson bracket* on the dual  $\mathfrak{g}^*$  of the Lie algebra  $\mathfrak{g}$ . Hamilton’s equations written in terms of a Lie–Poisson structure are called *Lie–Poisson systems*. Through the *momentum map*, they are closely related to the Hamiltonian equations on  $T^*G$ ,

where  $G$  is a Lie group (not necessarily finite-dimensional) for the corresponding Lie algebra  $\mathfrak{g}$ . The process of passing from Hamilton's equations on  $T^*G$  to the Lie–Poisson equations on  $\mathfrak{g}^*$  is called *Lie–Poisson reduction*, and the inverse process is called *Lie–Poisson reconstruction*. In this section, we address the main properties of such systems.

### 2.2.1 Adjoint and coadjoint representation

Let  $G$  be a Lie group, and  $\mathfrak{g}$  be its Lie algebra.

**Definition 2.8.** The map

$$A_g: G \rightarrow G, \quad A_g: h \mapsto ghg^{-1}$$

for  $g, h \in G$  is called an *inner automorphism*.

From now on, we will use the notation  $F_*|_x: T_xG \rightarrow T_{F(x)}G$  for the derivative of a map  $F: G \rightarrow G$ .

**Definition 2.9.** The differential of the inner automorphism at the unit element  $e$  of the group  $G$

$$\text{Ad}_g: \mathfrak{g} \rightarrow \mathfrak{g}, \quad \text{Ad}_g(u) = ((A_g)_*|_e)u, \quad u \in \mathfrak{g},$$

is called the *group adjoint operator*.

The property  $\text{Ad}_{gh} = \text{Ad}_g\text{Ad}_h$  implies that adjoint operators form a representation of the group  $G$  in its Lie algebra  $\mathfrak{g}$ , called the *adjoint representation*.

By differentiating  $\text{Ad}_g$  at the group unit element  $e$ , one gets the *adjoint representation of the Lie algebra  $\mathfrak{g}$* :

$$\text{ad} = \text{Ad}_{*e}: \mathfrak{g} \rightarrow \text{End}(\mathfrak{g}), \quad \text{ad}_v = \left. \frac{d}{dt} \right|_{t=0} \text{Ad}_{g(t)},$$

where  $g(t)$  is a curve on  $G$  passing through the unit element  $e \in G$  with the tangent vector  $v \in T_eG = \mathfrak{g}$ .

The following formula allows to express the  $\text{ad}$  operator in terms of the Lie bracket  $[\cdot, \cdot]$  on  $\mathfrak{g}$ :

$$\text{ad}_v(w) = [v, w], \quad v, w \in \mathfrak{g}.$$

Using the pairing  $\langle \cdot, \cdot \rangle$  between  $\mathfrak{g}$  and  $\mathfrak{g}^*$ , one can define the *coadjoint operator*:

$$\text{Ad}_g^*: \mathfrak{g}^* \rightarrow \mathfrak{g}^*, \quad \text{Ad}_g^*: \alpha \mapsto \text{Ad}_g^*(\alpha), \quad \langle \text{Ad}_g^*(\alpha), v \rangle = \langle \alpha, \text{Ad}_g v \rangle,$$

for any  $v \in \mathfrak{g}$ ,  $\alpha \in \mathfrak{g}^*$ ,  $g \in G$ .

As  $\text{Ad}_{gh}^* = \text{Ad}_h^*\text{Ad}_g^*$ , operators  $\text{Ad}_g^*$  form an *antirepresentation* of the group  $G$  in its coalgebra  $\mathfrak{g}^*$ .

**Definition 2.10.** The set of all points  $\text{Ad}_g^* \alpha$ ,  $g \in G$ , is called the *coadjoint orbit* of  $\alpha$ :

$$\mathcal{O}_\alpha = \{\text{Ad}_g^* \alpha \mid g \in G\}.$$

The dual operator for  $\text{ad}$ , the operator of the *coadjoint representation* is

$$\text{ad}_v^*: \mathfrak{g}^* \rightarrow \mathfrak{g}^*, \quad \langle \text{ad}_v^* \alpha, w \rangle = \langle \alpha, \text{ad}_v w \rangle,$$

for any  $v, w \in \mathfrak{g}$ ,  $\alpha \in \mathfrak{g}^*$ .

**Example 2.1.** Now we will illustrate the constructions introduced above for the group  $F = G \times \mathfrak{g}^*$ , which is called the *magnetic extension* of  $G$ . This group will be central in the context of incompressible magnetohydrodynamics.

We define the group  $F = G \times \mathfrak{g}^*$  as a set of pairs

$$F = \{(\phi, a) \mid \phi \in G, a \in \mathfrak{g}^*\}$$

with the group multiplication

$$(\phi, a) \cdot (\psi, b) = (\phi\psi, \text{Ad}_\psi^* a + b),$$

and  $(e, 0)$  being the unit element.

It can easily be verified that the inverse element is  $(\phi, a)^{-1} = (\phi^{-1}, -\text{Ad}_{\phi^{-1}}^* a)$ . Then, the formula for the inner automorphism is

$$\begin{aligned} A_{(\phi, a)}(\psi, b) &= (\phi, a) \cdot (\psi, b) \cdot (\phi, a)^{-1} = (\phi, a) \cdot (\psi, b) \cdot (\phi^{-1}, -\text{Ad}_{\phi^{-1}}^* a) = \\ &= (\phi\psi\phi^{-1}, \text{Ad}_{\psi\phi^{-1}}^* a + \text{Ad}_{\phi^{-1}}^* b - \text{Ad}_{\phi^{-1}}^* a). \end{aligned} \quad (2.13)$$

The Lie algebra of the group  $F$  is  $\mathfrak{f} = \mathfrak{g} \times \mathfrak{g}^*$ . Let us look for the adjoint operator on  $\mathfrak{f}$  in the form  $\text{ad}_{(v, \tilde{a})}(w, \tilde{b}) = (\xi, \eta)$ , where  $v, w, \xi \in \mathfrak{g}$ ,  $\tilde{a}, \tilde{b}, \eta \in \mathfrak{g}^*$ . Then, if the group elements  $(\phi, a)$  and  $(\psi, b)$  are generated in the neighborhood of the unit element as

$$\begin{aligned} \psi &= e + tw + o(t), & b &= t\tilde{b} + o(t), & w &\in \mathfrak{g}, & \tilde{b} &\in \mathfrak{g}^*, \\ \phi &= e + sv + o(s), & a &= s\tilde{a} + o(s), & v &\in \mathfrak{g}, & \tilde{a} &\in \mathfrak{g}^*, \end{aligned}$$

differentiating the first component in (2.13), we get

$$\xi = \left. \frac{d}{dt} \right|_{t=0} \left. \frac{d}{ds} \right|_{s=0} (\phi\psi\phi^{-1}) = vw - wv = [v, w].$$

Further, for the second component we get

$$\text{Ad}_{\psi\phi^{-1}}^* a + \text{Ad}_{\phi^{-1}}^* b - \text{Ad}_{\phi^{-1}}^* a = s\text{Ad}_{e-sv+tw}^* \tilde{a} + t\text{Ad}_{e-sv}^* \tilde{b} - s\text{Ad}_{e-sv}^* \tilde{a}.$$

Differentiating above expression, we get

$$\eta = \left. \frac{d}{dt} \right|_{t=0} \left. \frac{d}{ds} \right|_{s=0} (\text{Ad}_{\psi\phi^{-1}}^* a + \text{Ad}_{\phi^{-1}}^* b - \text{Ad}_{\phi^{-1}}^* a) = \text{ad}_w^* \tilde{a} - \text{ad}_v^* \tilde{b}.$$

Finally, we can write (we remove tildes, as it is not essential):

$$\text{ad}_{(v,a)}(w, b) = ([v, w], \text{ad}_w^* a - \text{ad}_v^* b).$$

Let us now obtain the expression for the coadjoint operator. To that end, we need to specify what the dual  $\mathfrak{f}^*$  is. We will identify the dual  $\mathfrak{f}^*$  with  $\mathfrak{f}$  itself,

$$\mathfrak{f}^* = \{(\xi, a) \mid \xi \in \mathfrak{g}, a \in \mathfrak{g}^*\},$$

with the pairing  $\langle\langle \cdot, \cdot \rangle\rangle$  defined as

$$\langle\langle (\xi, a), (\eta, b) \rangle\rangle = \langle b, \xi \rangle + \langle a, \eta \rangle, \quad (\xi, a) \in \mathfrak{f}^*, \quad (\eta, b) \in \mathfrak{f},$$

where  $\langle \cdot, \cdot \rangle$  is the standard pairing between  $\mathfrak{g}$  and  $\mathfrak{g}^*$ .

Using the definition of the coadjoint operator, we get

$$\begin{aligned} \langle\langle \text{ad}_{(v,a)}^*(\xi, \eta), (w, b) \rangle\rangle &= \langle\langle (\xi, \eta), \text{ad}_{(v,a)}(w, b) \rangle\rangle = \langle\langle (\xi, \eta), ([v, w], \text{ad}_w^* a - \text{ad}_v^* b) \rangle\rangle = \\ &= \langle \eta, [v, w] \rangle + \langle \text{ad}_w^* a - \text{ad}_v^* b, \xi \rangle = \langle \eta, \text{ad}_v w \rangle + \langle a, \text{ad}_w \xi \rangle - \langle b, \text{ad}_v \xi \rangle = \\ &= \langle \text{ad}_v^* \eta - \text{ad}_\xi^* a, w \rangle + \langle b, \text{ad}_\xi v \rangle = \langle \text{ad}_v^* \eta - \text{ad}_\xi^* a, w \rangle + \langle b, \text{ad}_\xi v \rangle = \\ &= \langle\langle (\text{ad}_\xi v, \text{ad}_v^* \eta - \text{ad}_\xi^* a), (w, b) \rangle\rangle. \end{aligned}$$

Finally, we arrive at the following formula for the coadjoint operator:

$$\text{ad}_{(v,a)}^*(w, b) = ([w, v], \text{ad}_v^* b - \text{ad}_w^* a).$$

## 2.2.2 Momentum maps and Lie–Poisson reduction

It is well known that the dynamics of a mechanical system with symmetries can be reduced to the dynamics on a manifold of smaller dimension, obtained as a quotient manifold by the symmetry group action. In the context of geometric mechanics, this observation can be formalized via the notion of a *momentum map*.

### Definition of the momentum map

Let  $(M, \{\cdot, \cdot\})$  be a Poisson manifold and let  $G$  be a Lie group acting on it:

$$\Phi: G \times M \rightarrow M, \quad (g, z) \mapsto \Phi_g(z) \in M \tag{2.14}$$

for any  $z \in M$  and  $g \in G$ .

Let us also assume that the action  $\Phi$  is canonical, i.e.

$$\Phi_g^* \{F_1, F_2\} = \{\Phi_g^* F_1, \Phi_g^* F_2\} \tag{2.15}$$

for any  $F_1, F_2 \in C^\infty(M)$ .

Let  $\mathfrak{g}$  be the Lie algebra of the Lie group  $G$ . Then, the action (2.14) is infinitesimally generated by the vector field  $\xi_M \in \mathcal{D}(M)$  induced by an element  $\xi \in \mathfrak{g}$ :

$$T_z M \ni \xi_M(z) = \left. \frac{d}{dt} \right|_{t=0} \exp(t\xi)(z). \quad (2.16)$$

We observe that

$$\Phi_{g^{-1}}^*(\xi_M) = (\text{Ad}_g \xi)_M. \quad (2.17)$$

Differentiating (2.17) at the neighborhood of the unit element,  $g(t) = e + t\eta + o(t^2)$ , we get an infinitesimal formulation of (2.17):

$$[\xi_M, \eta_M] = -[\xi, \eta]_M, \quad (2.18)$$

which implies that the map  $\xi \mapsto \xi_M$  is a Lie algebra *antihomomorphism*.

Condition (2.15) implies that

$$\xi_M(\{F_1, F_2\}) = \{\xi_M(F_1), F_2\} + \{F_1, \xi_M(F_2)\}, \quad (2.19)$$

that, however, does not mean that  $\xi_M$  is necessarily Hamiltonian. We will require that  $\xi_M$  is globally Hamiltonian, i.e.

$$\xi_M = X_{J(\xi)}$$

for some  $J(\xi) \in C^\infty(M)$ .

Infinitesimal formulation of a canonical action (2.15) yields that we have a *canonical Lie algebra action*  $\mathfrak{g} \ni \xi \mapsto \xi_M \in \mathcal{D}(M)$ , where  $\xi_M$  satisfies (2.19).

**Definition 2.11.** Let a Lie algebra  $\mathfrak{g}$  act canonically on a Poisson manifold  $M$ . Suppose there is a linear map  $J: \mathfrak{g} \rightarrow C^\infty(M)$ , such that

$$X_{J(\xi)} = \xi_M$$

for all  $\xi \in \mathfrak{g}$ . The map  $\mu: M \rightarrow \mathfrak{g}^*$  defined by

$$\langle \mu(z), \xi \rangle = J(\xi)(z)$$

for all  $\xi \in \mathfrak{g}$  and  $z \in M$ , is called a *momentum map*.

It is important to specify the construction of a momentum map for a subalgebra. Let  $\mathfrak{h} \subset \mathfrak{g}$  be a subalgebra, and assume that the action of  $\mathfrak{g}$  is canonical on  $M$ . Then,  $\mathfrak{h}$  also acts canonically on  $M$ . Assume also that  $\mu_{\mathfrak{g}}$  be the momentum map associated to the action of  $\mathfrak{g}$ . Then, action of  $\mathfrak{h}$  also admits a momentum map  $\mu_{\mathfrak{h}}: M \rightarrow \mathfrak{h}^*$  defined by

$$\mu_{\mathfrak{h}}(z) = \mu_{\mathfrak{g}}(z)|_{\mathfrak{h}}, \quad z \in M. \quad (2.20)$$

To show that, let us take  $\eta \in \mathfrak{h}$ . Then, since the  $\mathfrak{g}$  action admits a momentum map, and since also  $\eta \in \mathfrak{g}$ , we have  $\eta_M = X_{J_{\mathfrak{g}}(\eta)}$ . Therefore, putting  $J_{\mathfrak{h}}(\eta) = J_{\mathfrak{g}}(\eta)$  for all  $\eta \in \mathfrak{h}$  we define the induced  $\mathfrak{h}$ -momentum map. This is equivalent to

$$\langle \mu_{\mathfrak{h}}(z), \eta \rangle = \langle \mu_{\mathfrak{g}}(z), \eta \rangle$$

for all  $z \in M$ ,  $\eta \in \mathfrak{g}$ , which proves (2.20).

Thus in order to get a momentum map for a subalgebra action, one should compute the momentum map for an ambient algebra, and then project to the subalgebra.

**Example 2.2.** We will illustrate the concept of a momentum map and how to compute it again on the semidirect product group example, but at this time we will take the magnetic extension of one of the matrix Lie groups  $SU(N)$ , so that the group (previously denoted by  $G$ ) is  $F = SU(N) \ltimes \mathfrak{su}(N)^*$ . This group plays an important role in quantized MHD dynamics (see Paper I for more details).

Following the previous notation, we will specify the manifold  $M$  to be the total space of the cotangent bundle of  $F$ , i.e.  $M = T^*F = T^*(SU(N) \ltimes \mathfrak{su}(N)^*)$ . First, we clarify what  $T^*F$  is:

$$T^*F = \{(Q, m, P, \alpha) \mid Q \in SU(N), P \in T_Q^*(SU(N)), m \in \mathfrak{su}(N)^*, \alpha \in \mathfrak{su}(N)\}.$$

Consider the left action of  $F$  on  $T^*F$ :

$$(G, u) \cdot (Q, m, P, \alpha) = (GQ, \text{Ad}_Q^* u + m, (G^{-1})^\dagger P, \alpha) \quad (2.21)$$

for  $(G, u) \in F$ .

In order to find the corresponding momentum map (associated in this case to the left action)  $\mu: T^*F \rightarrow \mathfrak{f}^*$ , let us consider the infinitesimal action of  $F$  on  $T^*F$ . To that end, let  $(G, u)$  be close to the unit element:

$$\begin{aligned} G &= I + t\xi + o(t^2), & \xi &\in \mathfrak{su}(N), \\ u &= 0 + t\eta + o(t^2), & \eta &\in \mathfrak{su}(N)^*, \end{aligned}$$

thus, an infinitesimal generator is  $(\xi, \eta) \in \mathfrak{su}(N) \ltimes \mathfrak{su}(N)^*$ . Then, the infinitesimal left action will be

$$(G, u) \cdot (Q, m, P, \alpha) = (Q + t\xi Q + o(t^2), t\text{Ad}_Q^* \eta + m + o(t^2), P - t\xi^\dagger P + o(t^2), \alpha).$$

Differentiating above expression by  $t$  at  $t = 0$ , we get a vector field on  $M = T^*F$ :

$$\xi_{T^*F} = (\xi Q, \text{Ad}_Q^* \eta, -\xi^\dagger P, 0) = \left( \frac{\partial J}{\partial P}, \frac{\partial J}{\partial \alpha}, -\frac{\partial J}{\partial Q}, -\frac{\partial J}{\partial m} \right).$$

Solving this system of equations for the Hamiltonian  $J$ , we find

$$J = \text{tr}(P^\dagger \xi Q) + \text{tr}(\alpha^\dagger Q^\dagger \eta (Q^{-1})^\dagger) = \langle \mu, (\xi, \eta) \rangle,$$

and finally

$$\mu: T^*F \rightarrow \mathfrak{f}^*, \quad \mu(Q, m, P, \alpha) = (PQ^\dagger, Q\alpha Q^{-1}),$$

where we also used the pairing between  $\mathfrak{su}(N)$  and  $\mathfrak{su}(N)^*$  via the Frobenius inner product:

$$\langle A, B \rangle = \text{tr}(A^\dagger B), \quad A \in \mathfrak{su}(N)^*, \quad B \in \mathfrak{su}(N). \quad (2.22)$$

Note that we have not used so far that we work on a subalgebra  $\mathfrak{su}(N) \subset \mathfrak{gl}(N, \mathbb{C})$ . In particular, formula (2.22) does not guarantee that  $PQ^\dagger \in \mathfrak{su}(N)$ . As was discussed above, to get the final formula for the momentum map, we need to use an appropriate projector for (2.22) for the first component. That is not necessary for the second component, as it is an element of  $\mathfrak{su}(N)$  already. The only simplification we can make is to put  $Q^{-1} = Q^\dagger$ . Finally, the formula for the momentum map takes the form:

$$\mu(Q, m, P, \alpha) = \left( \frac{PQ^\dagger - QP^\dagger}{2}, Q\alpha Q^\dagger \right). \quad (2.23)$$

### Lie–Poisson structure on $\mathfrak{g}^*$ and Lie–Poisson reduction

Especially important is the case when the manifold  $M$  coincides with the total space of the cotangent bundle of the group  $G$  acting on it (exactly as in the previous example),  $M = T^*G$ .

First, one can consider the two natural actions of  $G$  on  $T^*G$ , left and right, that are the cotangent lifts of left or right action of  $G$  on itself. Then, identifying the set of smooth functions  $C^\infty(\mathfrak{g}^*)$  with the set of left (right) invariant functions on  $T^*G$ , one can obtain the Lie–Poisson bracket on  $\mathfrak{g}^*$ :

$$\{F, G\}_\pm(m) = \pm \left\langle m, \left[ \frac{\delta F}{\delta m}, \frac{\delta G}{\delta m} \right] \right\rangle, \quad (2.24)$$

where  $m \in \mathfrak{g}^*$ ,  $F, G \in C^\infty(\mathfrak{g}^*)$ , and the variational derivative  $\delta F/\delta m \in \mathfrak{g}$  is defined as

$$\frac{d}{d\varepsilon} \Big|_{\varepsilon=0} F(m + \varepsilon w) = \left\langle w, \frac{\delta F}{\delta m} \right\rangle, \quad w \in \mathfrak{g}^*.$$

The sign  $\pm$  in (2.24) is chosen to be  $+$  for right-invariant functions, and  $-$  for left-invariant.

The system of equations

$$\dot{F}(m(t)) = \{H, F\}_\pm(m(t)) \quad (2.25)$$

is called a *Lie–Poisson system*. The Hamiltonian function  $H \in C^\infty(\mathfrak{g}^*)$  is the conserved quantity, along with *Casimir functions*, i.e. functions  $C \in C^\infty(\mathfrak{g}^*)$ , such that  $\{C, \cdot\}_\pm = 0$ . Casimir functions are conserved quantities of (2.25) for any choice of the Hamiltonian function  $H$  and play an important role in structure

preserving numerical integration of (2.25), as their preservation by the numerical method is crucial for the long time dynamics.

Let us obtain a coadjoint representation of (2.25). For simplicity, we will choose the sign + and omit it. On the one hand, using the chain rule, we get

$$\dot{F}(m(t)) = \left\langle \dot{m}, \frac{\delta F}{\delta m} \right\rangle.$$

On the other hand,

$$\{H, F\} = \left\langle m, \left[ \frac{\delta H}{\delta m}, \frac{\delta F}{\delta m} \right] \right\rangle = \left\langle m, \text{ad}_{\frac{\delta H}{\delta m}} \frac{\delta F}{\delta m} \right\rangle = \left\langle \text{ad}_{\frac{\delta H}{\delta m}}^* m, \frac{\delta F}{\delta m} \right\rangle,$$

which implies that

$$\dot{m} = \text{ad}_{\frac{\delta H}{\delta m}}^* m. \quad (2.26)$$

Integrating (2.26) in time, we get

$$m(t) = \text{Ad}_{\exp(\int_0^t \frac{\delta H}{\delta m}(m(s)) ds)}^* m(0),$$

which drives us to a conclusion that the Lie–Poisson system (2.26) evolves on the coadjoint  $G$ -orbit of  $m(0) \in \mathfrak{g}^*$ , where the Casimir functions are constant. However, it is not always that Casimir functions completely define the coadjoint orbit.

A remarkable observation is that coadjoint orbits can be endowed with the symplectic structure.

**Theorem 2.5.** *Let  $G$  be a Lie group and let  $\mathcal{O} \subset \mathfrak{g}^*$  be a coadjoint orbit. Let also  $X, Y \in \mathfrak{g}$ . Then, there exist a symplectic form  $\omega$  on  $\mathcal{O}$  defined as*

$$\omega(\text{ad}_X^* m, \text{ad}_Y^* m)(m) = \langle m, [X, Y] \rangle \quad (2.27)$$

for all  $m \in \mathfrak{g}^*$ .

The symplectic form (2.27) is called *Kirillov–Kostant–Souriau form*. It is worth noting that (2.27) uses the identification  $T_m \mathfrak{g}^* \simeq \mathfrak{g}^*$  for all  $m \in \mathfrak{g}^*$ .

Finally, we conclude that the dual  $\mathfrak{g}^*$  is foliated by coadjoint orbits, each of which is a symplectic manifold, *symplectic leaf*.

Let us now establish relations between the Hamiltonian dynamics on  $T^*G$  and the Lie–Poisson dynamics on  $\mathfrak{g}^*$ . To this end, we will assume that the Hamiltonian function  $H$  on  $T^*G$  is left (right) invariant. Let also  $\mu_R$  and  $\mu_L$  be the momentum maps for the right and left action of  $G$  on  $T^*G$  respectively. Then, the *Lie–Poisson reduction theorem* says that the momentum map  $\mu_R$  ( $\mu_L$ ) reduces the Hamiltonian dynamics with the left (right) invariant Hamiltonian on  $T^*G$  to the Lie–Poisson dynamics (2.25) with the Hamiltonian  $H^-$  ( $H^+$ ) satisfying  $H = H^- \circ \mu_R$  ( $H =$

$H^+ \circ \mu_L$ ). If  $F_t$  is a flow of  $X_H$  on  $T^*G$ , then the corresponding flows  $F_t^\pm$  of  $X_{H^\pm}$  are related to  $F_t$  as

$$\begin{aligned}\mu_R(F_t(\alpha_g)) &= F_t^-(\mu_R(\alpha_g)) \\ \mu_L(F_t(\alpha_g)) &= F_t^+(\mu_L(\alpha_g)),\end{aligned}$$

where  $\alpha_g \in T_g^*G$ .

Inversely, having a Lie–Poisson system (2.26), one can lift the Hamiltonian  $H$  by means of left (right) momentum map, thus obtaining right (left) invariant Hamiltonian  $\tilde{H} = H \circ \mu_R$  (or  $\tilde{H} = H \circ \mu_L$ ). Then, equations (2.26) become canonical equations on  $T^*G$  with respect to  $H$ . This process is called *Lie–Poisson reconstruction*.

### Poisson property of the momentum map

Now we approach perhaps one of the most important property of the momentum map, which is the Poisson property.

Let us return to (2.18). Using that both maps  $\xi \mapsto \xi_M$  and  $H \mapsto X_H$  are Lie algebra antihomomorphisms, we obtain

$$X_{J([\xi, \eta])} = [\xi, \eta]_P = -[\xi_P, \eta_P] = -[X_{J(\xi)}, X_{J(\eta)}] = X_{\{J(\xi), J(\eta)\}}, \quad (2.28)$$

for all  $\xi, \eta \in \mathfrak{g}$ .

Note that (2.28) does not necessarily imply that

$$J([\xi, \eta]) = \{J(\xi), J(\eta)\} \quad (2.29)$$

Momentum maps that satisfy (2.29) are called *infinitesimally equivariant*.

**Theorem 2.6.** *Let  $\mu: M \rightarrow \mathfrak{g}^*$  be an infinitesimally equivariant momentum map for a left Hamiltonian action on a Poisson manifold  $M$ , then,  $\mu$  is a Poisson map:*

$$\mu^* \{F_1, F_2\}_+ = \{\mu^* F_1, \mu^* F_2\},$$

that is

$$\{F_1, F_2\}_+ \circ \mu = \{F_1 \circ \mu, F_2 \circ \mu\},$$

for all  $F_1, F_2 \in C^\infty(\mathfrak{g}^*)$ .

To prove the Poisson property, we will need the following

**Lemma 2.3.** *Let  $\mu: M \rightarrow \mathfrak{g}^*$  be an infinitesimally equivariant momentum map. Then,*

$$X_{F \circ \mu} = X_{J(\delta F / \delta m)} = \left( \frac{\delta F}{\delta m} \right)_M,$$

for any  $F \in C^\infty(\mathfrak{g}^*)$ .

*Proof.* Let us take any  $H \in C^\infty(\mathfrak{g}^*)$ , and let  $C^\infty(M) \ni \mu^*(F) = F \circ \mu$  be the pullback of  $F$ . Then,

$$\begin{aligned} X_{\mu^*(F)}(H) &= -X_H(\mu^*(F)) = -\langle d(\mu^*(F)), X_H \rangle = -\langle \mu^*(dF), X_H \rangle = \\ &= -\langle dF, \mu_*(X_H) \rangle = -\left\langle \mu_*(X_H), \frac{\delta F}{\delta m} \right\rangle, \end{aligned}$$

where in the last equality we used that  $\mu_*(X_H) \in \mathcal{D}(\mathfrak{g}^*)$  can be identified with  $\mathfrak{g}^*$  element. Further,

$$\begin{aligned} X_{\mu^*(F)}(H) &= -\left\langle \mu_*(X_H), \frac{\delta F}{\delta m} \right\rangle = -\left\langle d\left(J\left(\frac{\delta F}{\delta m}\right)\right), X_H \right\rangle = \\ &= -X_H\left(J\left(\frac{\delta F}{\delta m}\right)\right) = X_{J(\delta F/\delta m)}(H). \end{aligned}$$

□

Now we have all necessary ingredients to prove the Poisson property.

*Proof of Theorem 2.6.* Let  $z \in M$ , and  $m = \mu(z) \in \mathfrak{g}^*$ . Then,

$$\begin{aligned} \mu^* \{F, H\}_+ &= \{F, H\}_+(\mu(z)) = \left\langle \mu(z), \left[ \frac{\delta F}{\delta m}, \frac{\delta H}{\delta m} \right] \right\rangle = J\left(\left[ \frac{\delta F}{\delta m}, \frac{\delta H}{\delta m} \right]\right)(z) = \\ &= \left\{ J\left(\frac{\delta F}{\delta m}\right), J\left(\frac{\delta H}{\delta m}\right) \right\}(z) = X_{J(\delta H/\delta m)}\left(J\left(\frac{\delta F}{\delta m}\right)\right)(z) = X_{H \circ \mu}\left(J\left(\frac{\delta F}{\delta m}\right)\right) = \\ &= -X_{J(\delta F/\delta m)}(H \circ \mu)(z) = -X_{F \circ \mu}(H \circ \mu)(z) = \{F \circ \mu, H \circ \mu\}, \end{aligned}$$

which finalizes the proof. □

## 2.3 Geodesic equations on Lie groups

It was Euler himself who realized the basic concepts about fluid motion: it is a free motion of a large number of impenetrable particles in some fixed domain. In 1761, Euler [11] outlined a path toward understanding fluid dynamics, which, in modern terms, can be seen as follows: first, find a suitable configuration space  $M$  (i.e., sort out 'possible' motions from 'impossible' ones); second, formulate Newton's equations on  $M$  (i.e., select the one motion governed by mechanical principles). As one can see, already Euler had done a huge conceptual step forward to the modern understanding of fluids.

The next milestone in fluid mechanics (though it was not the main motivation) was the development of mechanics on finite-dimensional Lie groups originated from a 1901 two-page paper written by Poincaré [40]. Geometric mechanics allows to interpret motions of many mechanical systems as flows on finite-dimensional Lie groups, which serve as a configuration manifold for the corresponding mechanical

system. A prominent example is the rigid body with a fixed point, for which the group  $SO(3)$  is the configuration space. If the rigid body is free (no fixed points), the group becomes  $SE(3)$ . Another example is the Kirchhoff equations [28] describing a rigid body in a fluid.

Finally, in 1966, "standing on the shoulders of giants", Arnold [3] saw further than others: he realized that a leap from the finite-dimensional theory of Poincaré to infinite dimensions, along with Euler's concept of impenetrable particles, was possible, and formulated the incompressible Euler equations of hydrodynamics as Newton's equations on the group  $\text{Diff}_\mu(M)$  of volume-preserving diffeomorphisms, and thus making a significant progress in Euler's program 200 years later since the moment it was established.

It is hard to overestimate the importance of Arnold's discovery. His approach turned out to be universal: it has been shown to cover a wide variety of equations of mathematical physics ranging from incompressible and compressible fluids, magnetohydrodynamics, geophysical fluid dynamics, to Schrödinger and Camassa–Holm equations, optimal transport. Today, we refer to them as to *Euler–Arnold equations*. It gave a new breath to classical problems of fluid mechanics, such as stability of fluid motion, and well-posedness of the Euler equations [10].

Here, we discuss in detail the geodesic approach to fluids developed by Arnold.

### 2.3.1 Incompressible Euler's equations

Let  $(M, g)$  be a compact Riemannian manifold,  $\mu$  be the volume form associated with the metric  $g$ . If  $(x_1, \dots, x_n)$  are local coordinates on  $M$ , then  $\mu$  is

$$\mu = \sqrt{|\det(g_{ij}(x))|} dx_1 \wedge \dots \wedge dx_n.$$

Let  $\text{Diff}(M)$  be the group of diffeomorphisms of  $M$ ,  $\eta \in \text{Diff}(M)$ . We will assume that the manifold  $M$  is filled with an infinite number of particles of some liquid (gas). If at the moment  $t = 0$  a particle is located at the point  $x \in M$ , then at the current time moment it is located at the point  $\eta(x)$ . Let us define the tangent to  $\text{Diff}(M)$  space at the point  $\eta \in \text{Diff}(M)$  in the following way:

$$T_\eta \text{Diff}(M) = \{V \in C^\infty(M, TM) \mid V(x) = T_{\eta(x)}M, x \in M\}.$$

Here,  $C^\infty(M, TM)$  stands for the functions on  $M$  with values in the tangent space  $TM$ . Similarly to the finite-dimensional case, the Lie algebra  $\mathfrak{g}$  of the Lie group  $\text{Diff}(M)$  is defined as a tangent space at the neutral element  $e \in \text{Diff}(M)$  of the group,  $e(x) = x$ ,  $x \in M$ :

$$\mathfrak{g} = T_e \text{Diff}(M) = \{V \in C^\infty(M, TM) \mid V(x) = T_{e(x)}M = T_x M, x \in M\} = \mathcal{D}(M).$$

Thus, the Lie algebra  $\mathfrak{g}$  of the Lie group  $\text{Diff}(M)$  is a Lie algebra of vector fields on  $M$ .

The metric  $g$  on the manifold  $M$  induces an  $L^2$ -type metric on  $\text{Diff}(M)$  in the following way:

$$G_\eta(U, V) = \int_M g(U(x), V(x))\mu, \quad U, V \in T_\eta \text{Diff}(M), \eta \in \text{Diff}(M). \quad (2.30)$$

The physical interpretation of this metric is as follows: if  $V(x)$  is the velocity of a particle at the point  $\eta(x)$ , and the manifold  $M$  is filled with particles of the fluid, then  $\frac{1}{2}G_\eta(V, V)$  gives us the total kinetic energy of all the particles of the fluid.

It is known from physics that the motion of incompressible fluids is described by divergence-free vector fields, but the Lie algebra  $\mathfrak{g}$  that we constructed contains all vector fields. This means that one has to restrict the configuration space of incompressible fluids to the group  $\text{Diff}_\mu(M)$  of diffeomorphisms that preserve the volume element:

$$\text{Diff}_\mu(M) = \{\eta \in \text{Diff}(M) \mid \eta^*(\mu) = \mu\}.$$

Let us compute the corresponding Lie algebra  $\mathfrak{g} = T_e \text{Diff}_\mu(M)$ . Let  $\eta(t) \subset \text{Diff}_\mu(M)$  be a curve on a Lie group  $\text{Diff}_\mu(M)$  that goes through the neutral element  $e \in \text{Diff}_\mu(M)$ , and let  $v = \dot{\eta}(0)$ . Let us use that  $\eta(t)$  preserves the volume form  $\mu$ :

$$(\eta(t))^*(\mu) = \mu \Leftrightarrow \left. \frac{d}{dt} \right|_{t=0} (\eta(t))^*\mu = 0.$$

Since the left hand side of the equality is, by definition, the Lie derivative of  $\mu$  along the vector field  $v$ , we have

$$0 = L_v \mu = (\text{div}(v))\mu \Leftrightarrow \text{div}(v) = 0.$$

So the Lie algebra  $\mathfrak{g}$  of the Lie group of diffeomorphisms of  $M$  preserving the volume element consists of divergence-free vector fields on the manifold  $M$ , which means that the group  $\text{Diff}_\mu(M)$  is a suitable configuration space for incompressible fluids:

$$\mathfrak{g} = T_e \text{Diff}_\mu(M) = \mathcal{D}_\mu(M) = \{v \in \mathcal{D}(M) \mid \text{div}(v) = 0\}.$$

Let a curve  $\gamma: [0, 1] \rightarrow \text{Diff}_\mu(M)$  be a geodesic of the metric (2.30), that is an extremal of the functional

$$\tilde{S} = \int_0^1 \sqrt{G(\dot{\gamma}, \dot{\gamma})} dt = \int_0^1 dt \sqrt{\int_M g(\dot{\gamma}(x), \dot{\gamma}(x))\mu}. \quad (2.31)$$

If one chooses the unit velocity parametrization of the curve  $\gamma(t)$ , that is  $G(\dot{\gamma}, \dot{\gamma}) = 1$ , then extremizing the length functional (2.31) is equivalent to extremizing the energy functional

$$S = \frac{1}{2} \int_0^1 G(\dot{\gamma}, \dot{\gamma}) dt = \frac{1}{2} \int_0^1 dt \int_M g(\dot{\gamma}(x), \dot{\gamma}(x))\mu. \quad (2.32)$$

This can be shown by means of the Cauchy-Schwarz inequality

$$|(\varphi, \psi)|^2 \leq \|\varphi\|^2 \|\psi\|^2,$$

where  $\varphi(t), \psi(t) \in C[0, 1]$ , and scalar product is given by

$$\langle \varphi, \psi \rangle_{L^2} = \int_0^1 \varphi(t) \psi(t) dt.$$

Indeed, if one puts  $\varphi(t) = \sqrt{G(\dot{\gamma}, \dot{\gamma})}$ , and  $\psi(t) = 1$ , then one gets

$$\tilde{S}^2 \leq 2S,$$

with the equality if and only if  $\varphi = \psi$ , that is  $G(\dot{\gamma}, \dot{\gamma}) = 1$ . This means that finding extremals for (2.31) and (2.32) becomes equivalent, if  $G(\dot{\gamma}, \dot{\gamma}) = 1$ .

It is worth noting that from the mechanical viewpoint the functional (2.32) is the action functional for an incompressible fluid with the kinetic energy (Lagrangian)

$$\mathcal{L}(\dot{\gamma}, \dot{\gamma}) = \frac{1}{2} \int_M g(\dot{\gamma}(x), \dot{\gamma}(x)) \mu. \quad (2.33)$$

**Lemma 2.4.** *The Lagrangian (2.33) is right-invariant with respect to the group  $\text{Diff}_\mu(M)$ , that is*

$$\mathcal{L}(\dot{\gamma}, \dot{\gamma}) = \mathcal{L}(\dot{\gamma} \circ \eta, \dot{\gamma} \circ \eta), \quad \eta \in \text{Diff}_\mu(M). \quad (2.34)$$

*Proof.* It is sufficient to prove that the metric (2.30) is right-invariant, that is  $G(U \circ \eta, V \circ \eta) = G(U, V)$  for any  $\eta \in \text{Diff}_\mu(M)$ :

$$\begin{aligned} G(U \circ \eta, V \circ \eta) &= \int_M g((U \circ \eta)(x), (V \circ \eta)(x)) \mu = \int_M \underbrace{(g(U, V))}_{f} \circ \eta \mu = \\ &= \int_M (f \circ \eta) \eta^* \mu = \int_{\eta(M)} f \mu = \int_M f \mu = G(U, V), \end{aligned}$$

where we used the change of variables formula and the fact that  $\eta^* \mu = \mu$ .  $\square$

Note that the Riemannian metric (2.30) extended to the entire group  $\text{Diff}(M)$  is not right-invariant with respect to  $\text{Diff}(M)$ , but only with respect to its subgroup  $\text{Diff}_\mu(M)$ . Thus, compressible fluids, for which the configuration space is  $\text{Diff}(M)$ , is an example of a dynamical system on a Lie group where the symmetry group is smaller than the configuration space. It is important, because it means (in light of the Poisson reduction) that in the case of compressible Euler equations, it is impossible to reduce the dynamics of the fluid to the dynamics on the Lie algebra  $\mathcal{D}(M)$  of vector fields on  $M$ . One has to introduce also the time-dependent

density. However, it is still possible to find a configuration space for compressible fluids in a way that it serves also as a symmetry group (in other words, the entire configuration space is a symmetry group of the metric). This approach is based on introducing *semidirect product Lie groups*, and they often arise in the description of systems with broken symmetries. Examples of such systems include compressible fluids, and the two systems addressed in this thesis: magnetohydrodynamics and thermal quasi-geostrophic equations.

Let us turn back to functional (2.32). Since the Lagrangian is right-invariant, one can write (putting  $\eta = \gamma^{-1}$  in (2.34)):

$$S(v) = \frac{1}{2} \int_0^1 dt \int_M g(\dot{\gamma} \circ \gamma^{-1}, \dot{\gamma} \circ \gamma^{-1}) \mu = \frac{1}{2} \int_0^1 dt \int_M g(v, v) \mu, \quad (2.35)$$

where  $v = \dot{\gamma} \circ \gamma^{-1} \in \mathfrak{g}$ .

Taking the perturbation of the velocity  $v \mapsto v_\varepsilon$ , using that the curve  $\gamma(t)$  is a geodesic, i.e.

$$\left. \frac{d}{d\varepsilon} \right|_{\varepsilon=0} S(v_\varepsilon) = 0,$$

as well as Corollaries 2.4, 2.3, and Lemma 2.2, one gets the weak formulation of the incompressible Euler equation (see [34] for details):

$$0 = \int_0^1 \langle \dot{v} + \nabla_v v, u \rangle_{L^2} dt, \quad \text{for all } u \in \mathfrak{g} \quad (\operatorname{div}(u) = 0).$$

Since vector field  $u$  is divergence-free, but  $\dot{v} + \nabla_v v$ , in general, not, one cannot claim that  $\dot{v} + \nabla_v v = 0$ . We will use the following result (Helmholtz decomposition of vector fields):

**Theorem 2.7** (Helmholtz decomposition). *Let  $M$  be a compact manifold (possibly, with a boundary) and let  $u$  be a  $C^1$ -vector field on  $M$ . Then, there exist a  $C^1$ -vector field  $v$  and  $C^2$ -function  $f$ , such that*

$$u = v + \nabla f, \quad \operatorname{div}(v) = 0, \quad v|_{\partial M} = 0.$$

*Components  $v$  and  $\nabla f$  are  $L^2$ -orthogonal to each other:*

$$\langle v, \nabla f \rangle_{L^2} = \int_M (\nabla f \cdot v) \mu = 0.$$

Using the Helmholtz decomposition, we get

$$\dot{v} + \nabla_v v = -\nabla p.$$

Thus, the following theorem is proved:

**Theorem 2.8** (Arnold, [3]). *Let  $\gamma: [0, 1] \rightarrow \text{Diff}_\mu(M)$  be a geodesic of the Riemannian metric (2.30). Then, the vector field*

$$v(t) = \dot{\gamma}(t) \circ \gamma^{-1}(t)$$

*satisfies incompressible Euler's equations*

$$\dot{v} + \nabla_v v = -\nabla p, \quad \text{div}(v) = 0.$$

### 2.3.2 Newton's equations on $\text{Diff}(M)$

In this section, we will discuss a general formula for Newton's equations on the group of diffeomorphisms  $\text{Diff}(M)$  of some Riemannian manifold  $(M, g)$ , as well as their Hamiltonian version. We will use this formula to show universality of Arnold's approach to fluids. Namely, by choosing an appropriate potential energy function, we will show that the general form of Newton's equations transforms to Burger's equation, barotropic Euler's equations, and shallow water equation. Let, as before,  $\dim(M) = n$ , and  $\mu$  be the Riemannian volume form.

Let us start with the well-known Newton's equations on finite dimensional manifolds. If  $(M, g)$  is a Riemannian manifold, and  $\nabla$  is the Levi-Civita connection for the metric  $g$ , then, Newton's second law of mechanics ("acceleration=force") takes the form

$$\nabla_{\dot{q}} \dot{q} = -\nabla U(q), \tag{2.36}$$

where  $U(q)$  is the potential energy of a particle, and  $q(t) \in M$  is a curve on  $M$ . If the manifold  $M$  is flat, then (2.36) becomes  $\ddot{q} = -\nabla U(q)$ .

Let us now, following Arnold, make a leap from finite to infinite dimensions. Let  $\text{Dens}(M)$  be the space of smooth densities on  $M$  (by densities we mean either probability densities, that is positive smooth functions of  $n$  variables having the same total volume, or volume forms, which is equivalent). The group of diffeomorphisms  $\text{Diff}(M)$  is fibered over  $\text{Dens}(M)$  in the following way: a fiber over  $\mu$  is a subgroup  $\text{Diff}_\mu(M)$ , while a fiber over the volume form  $\tilde{\mu}$  consists of all diffeomorphisms  $\varphi$ , such that  $\varphi_*\mu = \tilde{\mu}$ , or, equivalently,  $\text{Jac}(\varphi^{-1})\mu = \tilde{\mu}$  (Due to the Moser's theorem diffeomorphisms from the group  $\text{Diff}(M)$  act transitively on densities [39]). In other words, two diffeomorphisms  $\varphi_1$  and  $\varphi_2$  belong to the same fiber, if  $\varphi_1 = \varphi_2 \circ \phi$  for some  $\phi \in \text{Diff}_\mu(M)$ . Analogously to (2.36), one can introduce Newton's equations on the infinite-dimensional group  $\text{Diff}(M)$ .

**Definition 2.12.** Newton's equations on the group  $\text{Diff}(M)$  are equations of the form

$$\nabla_{\dot{\varphi}}^G \dot{\varphi} = -\nabla^G U(\varphi),$$

where  $U: \text{Diff}(M) \rightarrow \mathbb{R}$  is the potential function,  $\nabla^G$  is the covariant derivative, associated with the metric  $G$ .

We shall consider potentials that depend on  $\varphi$  via density:  $U(\varphi) = \bar{U}(\rho)$ , where  $\rho = \text{Jac}(\varphi^{-1})$ , i.e.  $\varphi_*\mu = \rho\mu$ .

**Theorem 2.9** ([44, 45]). *Newton's equations on the group  $\text{Diff}(M)$  can be written in the form*

$$\nabla_{\dot{\varphi}}\dot{\varphi} = - \left( \nabla \frac{\delta \bar{U}}{\delta \rho} \right) \circ \varphi, \quad (2.37)$$

where  $\nabla$  is the covariant derivative, associated with the metric  $g$ , and  $\frac{\delta \bar{U}}{\delta \rho}$  is the variational derivative of the potential  $\bar{U}$ .

Formula (2.37) allows to express Newton's equations on  $\text{Diff}(M)$  in terms of differential geometric operations on  $M$ .

### Hamiltonian form of Newton's equations

In this section, we will get several equations of fluid mechanics as Hamiltonian systems on  $T^*\text{Diff}(M)$ . To this end, we first identify the cotangent space  $T^*_\varphi\text{Diff}(M)$  with the dual to the space of vector fields:  $\mathcal{D}^*(M) = T^*_{\text{id}}\text{Diff}(M)$ , which consists of differential 1-forms with values in densities:

$$\mathcal{D}^*(M) = \Omega^1(M) \otimes \text{Dens}(M).$$

The natural pairing between  $\dot{\varphi} \in T_\varphi\text{Diff}(M)$  and  $m = \alpha \otimes \mu \in T^*_\varphi\text{Diff}(M)$  is given by the formula

$$\langle m, \dot{\varphi} \rangle_\varphi = \int_M \iota_{\dot{\varphi} \circ \varphi^{-1}} m = \int_M (\iota_{\dot{\varphi} \circ \varphi^{-1}} \alpha) \mu.$$

The Lagrangian on  $T\text{Diff}(M)$  is of the form

$$\mathcal{L}(\varphi, \dot{\varphi}) = \frac{1}{2} G_\varphi(\dot{\varphi}, \dot{\varphi}) - \bar{U}(\varphi_*\mu). \quad (2.38)$$

It is known that the transition from the Lagrangian formulation to the Hamiltonian one is performed by means of the Legendre transformation:

$$m = v^b \otimes \varrho, \quad \text{where } v = \dot{\varphi} \circ \varphi^{-1}, \quad \varrho = \varphi_*\mu,$$

where  $v^b \in \Omega^1(M)$ ,  $v^b(u) = g(v, u)$ ,  $u \in \mathcal{D}(M)$ .

**Lemma 2.5.** *The Hamiltonian corresponding to the Lagrangian (2.38) is*

$$H(\varphi, m) = \frac{1}{2} \langle m, v \rangle + \bar{U}(\varphi_*\mu).$$

**Theorem 2.10** ([27]). *The Hamiltonian form of equations (2.37) is*

$$\begin{cases} \dot{m} = -L_v m + d \left( \frac{1}{2} |v|^2 - \frac{\delta \bar{U}}{\delta \varrho}(\varphi_*\mu) \right) \otimes \varphi_*\mu, \\ \dot{\varphi} = v \circ \varphi, \end{cases} \quad (2.39)$$

where  $m = v^b \otimes \varphi_*\mu$ .

*Remark 2.5.* Equations (2.39) can be obtained by using the Poisson form of the canonical equations

$$\dot{F} = \{H, F\},$$

where  $F(\varrho, m) = \langle m, u \rangle + \langle \varrho, \theta \rangle$ ,  $u \in \mathcal{D}$ ,  $\theta \in C^\infty(M)$ , and  $\{F, G\}$  is the Lie-Poisson bracket on  $T^*\text{Diff}(M)$ , that is generally given by

$$\{F, G\}(\xi) = \left\langle \xi, \left[ \frac{\delta F}{\delta \xi}, \frac{\delta G}{\delta \xi} \right] \right\rangle, \quad \xi \in T^*\text{Diff}(M).$$

In our case it has the form

$$\{F, G\}(\varrho, m) = \left\langle \varrho, L_{\frac{\delta F}{\delta m}} \frac{\delta G}{\delta \varrho} - L_{\frac{\delta G}{\delta m}} \frac{\delta F}{\delta \varrho} \right\rangle + \left\langle m, L_{\frac{\delta F}{\delta m}} \frac{\delta G}{\delta m} \right\rangle. \quad (2.40)$$

Let us now obtain equations (2.39) in a more familiar form, the velocity–density formulation. First, we get the flow equation on densities. We use that  $\rho\mu = \varphi_*\mu = (\varphi_t^*)^{-1}\mu$ , which implies that  $\mu = \varphi_t^*(\rho\mu)$ . Differentiating this expression with respect to  $t$ , putting  $t = 0$  and using that  $\varphi_t$  is the flow of  $v$ , we get

$$0 = \frac{d}{dt}(\varphi_t^*(\rho)\varphi_t^*(\mu)) = \left( \frac{d}{dt}\varphi_t^*(\rho) \right) \varphi_t^*(\mu) + \varphi_t^*(\rho) \frac{d}{dt}\varphi_t^*(\mu). \quad (2.41)$$

Let us now use the formula

$$\frac{d}{dt}\varphi_t^*\alpha = \varphi_t^*(L_v\alpha).$$

One has to take into account that in the expression  $\frac{d}{dt}\varphi_t^*(\rho)$  the dependence on  $t$  is present in two places:  $\rho$  depends on  $t$ , and the flow itself is evaluated at the point  $t$ . So,

$$\frac{d}{dt}\varphi_t^*(\rho) = \varphi_t^*(\dot{\rho}) + \varphi_t^*(L_v\rho) = \varphi_t^*(\dot{\rho} + L_v\rho).$$

Let us turn back to (2.41):

$$0 = \varphi_t^*(\dot{\rho} + L_v\rho)\varphi_t^*(\mu) + \varphi_t^*(\rho)L_v\mu = \varphi_t^*(\dot{\rho}\mu + L_v(\rho\mu)),$$

which implies that

$$\dot{\rho} + \text{div}(\rho v) = 0. \quad (2.42)$$

Equation (2.42) is the well-known *continuity equation* of fluid mechanics reflecting the conservation of mass. We note that for incompressible fluids, i.e. for those with  $\rho = \text{const}$ , equation (2.42) reduces to  $\text{div}(v) = 0$ .

Further, since  $m = v^b \otimes \varrho$ , then

$$\dot{m} = \rho \dot{v}^b \otimes \mu + \dot{\rho} v^b \otimes \mu. \quad (2.43)$$

Consider the action of the Lie derivative on  $m$  in more details:

$$L_v m = L_v(v^b \otimes \rho\mu) = (L_v v^b) \otimes \rho\mu + v^b \otimes L_v(\rho\mu) = \rho(L_v v^b) \otimes \mu + \text{div}(\rho v) v^b \otimes \mu.$$

Using the equation for  $m$  in (2.39) and (2.43), one can write

$$\rho \dot{v}^b \otimes \mu + \dot{\rho} v^b \otimes \mu = -\rho (L_v v^b) \otimes \mu - \underbrace{\operatorname{div}(\rho v)}_{\dot{\rho}} v^b \otimes \mu + \rho d \left( \frac{1}{2} |v|^2 \right) \otimes \mu - \rho \left( d \frac{\delta \bar{U}}{\delta \rho} \right) \otimes \mu.$$

Simplifying, we get

$$\dot{v}^b \otimes \mu = -(L_v v^b) \otimes \mu + d \left( \frac{1}{2} |v|^2 \right) \otimes \mu - \left( d \frac{\delta \bar{U}}{\delta \rho} \right) \otimes \mu. \quad (2.44)$$

Using the result Lemma 2.2, one can write (2.44) as follows:

$$\left( \dot{v}^b + \frac{1}{2} d |v|^2 + (\nabla_v v)^b - d \left( \frac{1}{2} |v|^2 \right) + \left( d \frac{\delta \bar{U}}{\delta \rho} \right) \right) \otimes \mu = 0.$$

Using that the volume form  $\mu$  is non-degenerate and applying the sharp operator  $\sharp$  we get

$$\dot{v} + \nabla_v v = -\nabla \frac{\delta \bar{U}}{\delta \rho}. \quad (2.45)$$

Consider a few particular cases of equation (2.45).

**Example 2.3** (Burgers equation). In case of  $\bar{U} = 0$  equation (2.45) takes the form of the Burgers equation

$$\dot{v} + \nabla_v v = 0.$$

**Example 2.4** (Barotropic Euler equations). Barotropic fluids are fluids with the pressure function depending solely on the density  $\rho$ :  $P = P(\rho)$ . The potential energy  $\bar{U}(\rho)$  is

$$\bar{U}(\rho) = \int_M \Phi(\rho) \mu,$$

where  $\Phi(\rho)$  is related to  $P(\rho)$  as:  $\Phi'' = \rho^{-1} P'$ . Thus, equation (2.45) becomes

$$\dot{v} + \nabla_v v = -\rho^{-1} \nabla P(\rho).$$

**Example 2.5** (Shallow water equations). In case  $\bar{U}(\rho) = \frac{1}{2} \int_M \rho^2 \mu$  we get the shallow water equations:

$$\dot{v} + \nabla_v v + \nabla \rho = 0.$$

### 2.3.3 Incompressible MHD as a Lie–Poisson system

Here, we use the abstract constructions introduced previously to show the Hamiltonian structure of incompressible magnetohydrodynamics. Namely, we show that the system of self-consistent incompressible magnetohydrodynamics is a Lie–Poisson system on the dual  $\mathfrak{im}\mathfrak{h}^*$  of the semidirect product Lie algebra  $\mathfrak{im}\mathfrak{h} =$

$\mathcal{D}_\mu(M) \times (\Omega^1(M)/d\Omega^0(M))$ . Informally speaking, the first component is responsible for the velocity field, and the second one stands for the magnetic field.

The system reads

$$\begin{cases} \dot{v} + \nabla_v v = -\nabla p + \text{curl} B \times B, \\ \dot{B} = L_v B, \\ \text{div} B = 0, \\ \text{div} v = 0. \end{cases} \quad (2.46)$$

Here,  $B(t, x)$  is the divergence-free magnetic field,  $v(t, x)$  is the divergence-free velocity field,  $p(t, x)$  is a pressure function,  $L_v$  denotes the Lie derivative along the vector field  $v(t, x)$ , and  $\nabla_v v$  is the covariant derivative of the vector field  $v$  along itself,  $x \in M$ .

We start with the configuration space for MHD, which is the *magnetic extension* of the Lie group of volume-preserving diffeomorphisms  $\text{Diff}_\mu(M)$ :

$$\text{IMH} = \text{Diff}_\mu(M) \times (\Omega^1(M)/d\Omega^0(M)),$$

where the subscript  $\mu$  stands for the Riemannian volume form on  $M$  for the given Riemannian metric  $g$  on  $M$ .

The corresponding Lie algebra of the Lie group IMH is

$$\mathfrak{imh} = \mathcal{D}_\mu(M) \times (\Omega^1(M)/d\Omega^0(M)),$$

and its dual is

$$\mathfrak{imh}^* = \mathcal{D}_\mu^*(M) \oplus \mathcal{D}_\mu(M) \simeq \mathcal{D}_\mu^*(M) \oplus \Omega_{\text{cl}}^2(M).$$

Magnetic fields  $B \in \mathcal{D}_\mu(M)$  can be identified with closed differential 2-forms  $\beta \in \Omega_{\text{cl}}^2(M)$  by the following way:

$$\iota_B \mu = \beta.$$

In other words,

$$\mathfrak{imh}^* = \left\{ (m, B) \mid m = v^\flat \otimes \mu, B \in \mathcal{D}_\mu(M) \right\}.$$

The pairing between  $\mathfrak{imh}$  and  $\mathfrak{imh}^*$  is given as follows:

$$\langle (v, \alpha), (m, B) \rangle = \int_M (\iota_v v^\flat) \mu + \int_M (\iota_B \alpha) \mu = \langle B, \alpha \rangle + \langle m, v \rangle.$$

The energy of a charged fluid is a sum of its kinetic energy and the energy of a magnetic field, and therefore the Hamiltonian of an incompressible charged fluid has the following form:

$$H = \frac{1}{2} \int_M (|m|^2 + |B|^2) \mu.$$

The Lie–Poisson equations on  $\mathfrak{mh}^*$  are

$$\dot{F} = \{H, F\},$$

where the expression for the Lie–Poisson bracket  $\{\cdot, \cdot\}$  is given by (2.24) interpreted accordingly. Indeed, for any  $(m, B) \in \mathfrak{mh}^*$

$$\{F, G\}(m, B) = \left\langle m, L_{\frac{\delta F}{\delta m}} \frac{\delta G}{\delta m} \right\rangle + \left\langle B, L_{\frac{\delta G}{\delta m}} \frac{\delta F}{\delta B} - L_{\frac{\delta F}{\delta m}} \frac{\delta G}{\delta B} \right\rangle.$$

Taking  $F(m, B) = \langle m, u \rangle + \langle B, \theta \rangle$  for some  $u \in \mathcal{D}_\mu(M)$  and  $\theta \in \mathcal{D}_\mu^*(M) \simeq \Omega^1(M)/d\Omega^0(M)$ , we get

$$\dot{F} = \langle \dot{m}, u \rangle + \langle \dot{B}, \theta \rangle = \{H, F\} = \langle m, L_v u \rangle + \langle B, L_u \mathcal{B} \rangle - \langle B, L_v \theta \rangle, \quad (2.47)$$

where  $\mathcal{B} = B^\flat \otimes \mu$ . We will need a number of lemmas.

**Lemma 2.6.**  $\langle m, L_v u \rangle = -\langle L_v m, u \rangle$ .

*Proof.*

$$-\langle L_v m, u \rangle = -\int_M \iota_u(L_v m) = -\int_M \iota_u \left( (L_v v^\flat) \otimes \mu + v^\flat \otimes L_v \mu \right)$$

Since  $L_v \mu = (\operatorname{div}(v))\mu = 0$ , we get

$$\begin{aligned} -\langle L_v m, u \rangle &= -\int_M (L_v v^\flat)(u)\mu = -\int_M (v(g(v, u)) - g(v, [v, u]))\mu = \\ &= \int_M g(v, L_v u)\mu - \int_M v(g(v, u))\mu = \langle m, L_v u \rangle - \int_M v(g(u, v))\mu. \end{aligned}$$

Let us consider the last integral in more details.

$$\begin{aligned} \int_M v(g(u, v))\mu &= \int_M L_v(g(v, u))\mu = \int_M L_v(g(v, u)\mu) - \int_M g(v, u)L_v \mu = \\ &= \int_M \operatorname{div}(vg(v, u))\mu = \int_{\partial M} (v \cdot n)g(v, u)\mu = 0, \end{aligned}$$

since  $v$  is tangent to the boundary. □

**Lemma 2.7.**  $\langle B, L_u \mathcal{B} \rangle = \langle L_B \mathcal{B}, u \rangle$ .

*Proof.*

$$\langle B, L_u \mathcal{B} \rangle = \int_M \iota_B(L_u B^\flat)\mu = \int_M (B(g(B, u)) - g(B, [B, u]))\mu = -\langle \mathcal{B}, L_B u \rangle \quad (2.48)$$

by the same reasons as in the previous lemma.

$$\langle L_B \mathcal{B}, u \rangle = \int_M (L_B \mathcal{B})(u) \mu = \int_M B(B^b(u)) \mu - \int_M B^b([B, u]) \mu = -\langle \mathcal{B}, L_B u \rangle, \quad (2.49)$$

where we used the same ideas as in the previous lemma. Finally, from (2.48) and (2.49), we get  $\langle B, L_u \mathcal{B} \rangle = \langle L_B \mathcal{B}, u \rangle$ .  $\square$

**Lemma 2.8.**  $\langle B, L_v \theta \rangle = -\langle L_v B, \theta \rangle$ .

*Proof.*

$$\langle B, L_v \theta \rangle = \int_M \iota_B(L_v \theta) \mu = \int_M (L_v \theta)(B) \mu = \int_M (v(\theta(B)) - \theta([v, B])) \mu = -\langle L_v B, \theta \rangle.$$

$\square$

Using results of these three lemmas, we can write down (2.47) as follows:

$$\langle \dot{m}, u \rangle + \langle \dot{B}, \theta \rangle = -\langle L_v m, u \rangle + \langle L_B \mathcal{B}, u \rangle + \langle L_v B, \theta \rangle,$$

and we conclude that incompressible MHD equations are

$$\begin{cases} \dot{m} = -L_v m + L_B \mathcal{B}, \\ \dot{B} = L_v B, \\ \operatorname{div} B = 0, \operatorname{div}(v) = 0. \end{cases} \quad (2.50)$$

It is important to get the first equation in terms of the velocity field  $v$ . To this end, let us take the first equation in (2.50) and apply the sharp operator  $\sharp$ :

$$(\dot{m} + L_v m - L_B \mathcal{B})^\sharp = \left( \dot{v}^b + L_v v^b - L_B B^b \right)^\sharp \otimes \mu.$$

Using the result of Lemma 2.2, we get

$$\left( L_v v^b \right)^\sharp = \nabla_v v + \nabla P_1$$

for some function  $P_1(t, x)$ .

One can verify that

$$\left( L_B B^b \right)^\sharp = \operatorname{curl} B \times B + \nabla |B|^2,$$

and finally we end up with

$$\dot{v} + \nabla_v v + \nabla P = \operatorname{curl} B \times B, \quad (2.51)$$

for some function  $P(t, x)$ , and (2.51) now coincides with the first equation in (2.46).



### 3 Numerical methods for Hamiltonian and Lie–Poisson systems

The basic idea that stands behind the *geometric numerical integration* is to preserve the properties of an exact equation by a numerical method. For example, if some equation (or system of equations) has conservation laws, then the numerical method that is used to solve this equation approximately, must preserve those conservation laws. More generally, if there are geometric structures underlying a PDE, then the method must preserve these structures. The importance of preserving the geometrical properties is outlined in the first chapter of the book [15], where numerous examples that demonstrate a better reliability of geometric integrators are provided.

Here, we discuss some approaches to construction of geometric integrators for Hamiltonian and Lie–Poisson systems.

#### 3.1 Motivation for structure preservation

Let us start with a demonstration of the superiority of geometric integrators over non-geometric ones when applied to a Hamiltonian system. We show that preservation of conserved quantities (such as, for example, the Hamiltonian) of the exact flow provides a more accurate qualitative long time dynamics. As an example, we will use Hamilton’s equations for *molecular dynamics*.

Consider the model describing interaction between particles in some medium (for example, liquid or gas) on the plane. Assume that there are  $N$  particles located at positions  $\mathbf{q}_i = (q_i^1, q_i^2)$  and having momenta  $\mathbf{p}_i = (p_i^1, p_i^2)$ ,  $i = 1, \dots, N$ . Then, the Hamiltonian will have the form

$$H(\mathbf{p}, \mathbf{q}) = \sum_{i=1}^N \frac{1}{2} \|\mathbf{p}_i\|^2 + \sum_{i=1}^N \sum_{j>i}^N V(\|\mathbf{q}_i - \mathbf{q}_j\|), \quad (3.1)$$

where the interaction potential  $V(r)$  is the Lennard–Jones potential

$$V(r) = \frac{1}{r^{12}} - \frac{2}{r^6}.$$

We will simulate the Hamiltonian dynamics

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial q_i}, \quad i = 1, \dots, N,$$

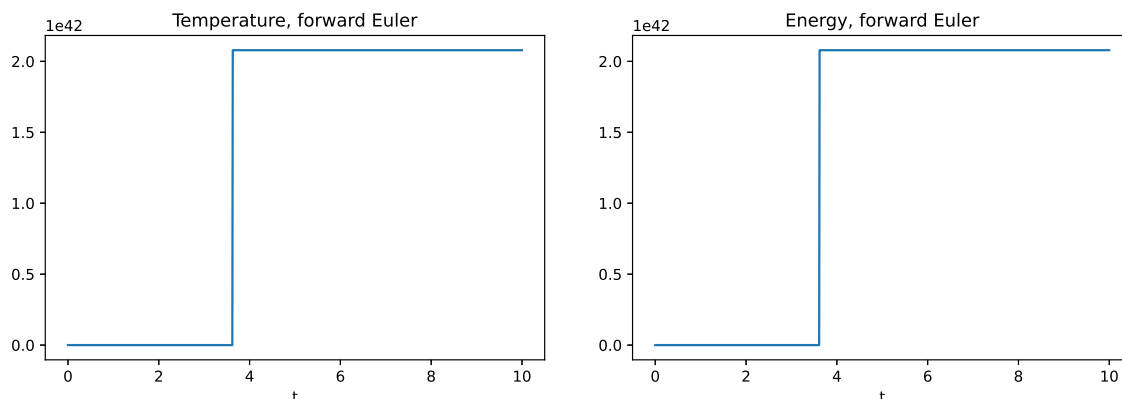
with the Hamiltonian given by (3.1) using the forward Euler method, which is a non-symplectic first order method, and Störmer–Verlet method, which is a symplectic method of order 2. For a system of ODEs  $\dot{y} = f(y)$ ,  $y \in \mathbb{R}^n$ , the forward Euler method is formulated as

$$y_{n+1} = y_n + hf(y_n),$$

and the Störmer–Verlet method as (for a Hamiltonian system)

$$\begin{aligned} p_{n+1/2} &= p_n - \frac{h}{2} H_q(p_{n+1/2}, q_n), \\ q_{n+1} &= q_n + \frac{h}{2} (H_p(p_{n+1/2}, q_n) + H_p(p_{n+1/2}, q_{n+1})), \\ p_{n+1} &= p_{n+1/2} - \frac{h}{2} H_q(p_{n+1/2}, q_{n+1}). \end{aligned}$$

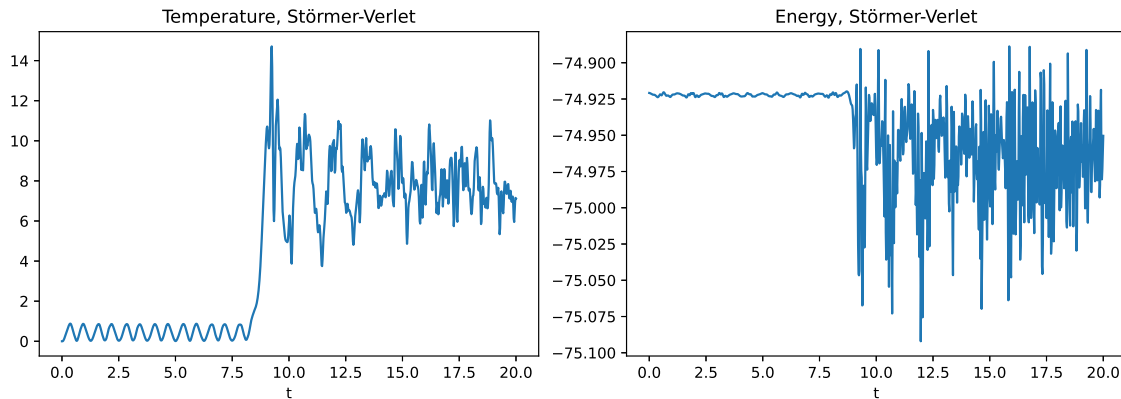
First, we provide simulation results obtained by the forward Euler method with the step size  $h = 0.01$ . One can see from Fig. 3.1 that the forward Euler



**Fig. 3.1.** Simulation results for molecular dynamics with  $N = 36$  molecules. Temperature (left) and energy (right) for the forward Euler method with the step size  $h = 0.01$ .

method produces absolutely incorrect results with energy and temperature being of magnitude  $10^{42}$  after a certain time moment.

Further, we provide simulation results obtained by the Störmer–Verlet method with the step size  $h = 0.02$ . The Störmer–Verlet method performs much better even for a larger step size  $h = 0.02$  compared to the forward Euler method. Energy is nearly conserved up until a certain time moment  $t \approx 10$ , where one observes a jump in temperature and higher oscillations in energy. This indicates the presence



**Fig. 3.2.** Simulation results for molecular dynamics with  $N = 36$  molecules. Temperature (left) and energy (right) for the Störmer–Verlet method with the step size  $h = 0.02$ .

of a phase transition — a transformation of a medium from liquid to gas phase (or vice versa).

Clearly, symplectic integrator provides much more reliable results compared to the forward Euler scheme that blows up even for a smaller time stepping.

## 3.2 Symplectic integration of Hamiltonian systems

As was outlined previously, one of the main properties of Hamiltonian systems

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial q_i}, \quad i = 1, \dots, n, \quad (3.2)$$

is symplecticity.

Let  $(p^{(k)}, q^{(k)})$  be the values of unknowns  $p(t), q(t)$  at the discrete time moment  $t_k$ . If  $\Phi_h: (p^{(k)}, q^{(k)}) \mapsto (p^{(k+1)}, q^{(k+1)})$ , is a numerical scheme for (3.2) with  $h$  being the time stepping, then the condition for it to be symplectic can be expressed as

$$dp^{(k)} \wedge dq^{(k)} = dp^{(k+1)} \wedge dq^{(k+1)}, \quad (3.3)$$

so the canonical symplectic form  $\Omega = dp \wedge dq$  is invariant under  $\Phi_h$ .

Given a Butcher tableau

$$\begin{array}{c|cccc} c_1 & a_{11} & a_{12} & \cdots & a_{1s} \\ c_2 & a_{21} & a_{22} & \cdots & a_{2s} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & a_{s2} & \cdots & a_{ss} \\ \hline & b_1 & b_2 & \cdots & b_s \end{array}$$

with  $c_i = \sum_{j=1}^s a_{ij}$ , the corresponding  $s$ -stage *Runge-Kutta* method for an ODE (system of ODEs)  $\dot{y} = f(t, y)$  is defined as

$$y_{n+1} = y_n + h \sum_{i=1}^s b_i k_i, \quad k_i = f \left( t_n + c_i h, y_n + h \sum_{j=1}^s a_{ij} k_j \right), \quad i = 1, \dots, s. \quad (3.4)$$

**Theorem 3.1** ([42]). *If  $b_i a_{ij} + b_j a_{ji} = b_i b_j$  for all  $j = 1, \dots, s$ , then the Runge-Kutta method (3.4) is symplectic.*

The simplest example of a symplectic Runge-Kutta method is the *implicit midpoint method*:

$$\begin{cases} q^{(k)} = \tilde{q} - \frac{h}{2} H_p(\tilde{p}, \tilde{q}), & q^{(k+1)} = \tilde{q} + \frac{h}{2} H_p(\tilde{p}, \tilde{q}), \\ p^{(k)} = \tilde{p} + \frac{h}{2} H_q(\tilde{p}, \tilde{q}), & p^{(k+1)} = \tilde{p} - \frac{h}{2} H_q(\tilde{p}, \tilde{q}). \end{cases} \quad (3.5)$$

One can show symplecticity of the midpoint method (3.5) by checking the equality (3.3). On the one hand,

$$dp^{(k)} \wedge dq^{(k)} = d\tilde{q} \wedge d\tilde{p} - \frac{h^2}{4} H_{pp}(\tilde{p}, \tilde{q}) H_{qq}(\tilde{p}, \tilde{q}) d\tilde{q} \wedge d\tilde{p} - \frac{h^2}{4} H_{pq}^2(\tilde{p}, \tilde{q}) d\tilde{p} \wedge d\tilde{q}. \quad (3.6)$$

On the other hand, using the left part of the method, we get

$$dp^{(k+1)} \wedge dq^{(k+1)} = d\tilde{q} \wedge d\tilde{p} - \frac{h^2}{4} H_{pp}(\tilde{p}, \tilde{q}) H_{qq}(\tilde{p}, \tilde{q}) d\tilde{q} \wedge d\tilde{p} - \frac{h^2}{4} H_{pq}^2(\tilde{p}, \tilde{q}) d\tilde{p} \wedge d\tilde{q}. \quad (3.7)$$

Clearly, the right hand sides of (3.6) and (3.7) coincide.

### 3.3 Geometric integration of Poisson systems

For Poisson systems the problem of finding an integrator that respects the underlying geometric properties is more complicated. In particular, a symplectic Runge-Kutta scheme, in general, does not yield a Lie–Poisson integrator when directly applied to a Lie–Poisson system.

Existing approaches to constructing Lie–Poisson integrators include, for instance, *splitting methods* [32, 33]. They are used if the Hamiltonian can be decomposed into a sum of integrable Hamiltonians. The other approach is to use the constrained integrator RATTLE [8]. One lifts the equations on  $\mathfrak{g}^*$  to  $T^*G$  and then solves a constrained Hamiltonian system. Most of the methods result in computationally expensive and complicated schemes, involving exponential maps and group to algebra maps.

In the framework of the Lie–Poisson reduction described in the previous chapter, it is natural to develop a *discrete Lie–Poisson reduction*. The idea is to utilize the properties of the momentum map  $\mu: T^*G \rightarrow \mathfrak{g}^*$ , such as the Poisson property, and symplecticity of the Runge-Kutta scheme [36]. Indeed, having a discrete symplectic map provided by the symplectic Runge-Kutta integrator, that is also left (right) invariant, one reduces it to a Lie–Poisson integrator on  $\mathfrak{g}^*$ . The integrators obtained via the discrete Lie–Poisson reduction (see, for example, [36] and Paper I of the present thesis)

- are formulated explicitly on  $\mathfrak{g}^*$ ;
- do not require computation of expensive maps (matrix multiplication is the most expensive operation);
- are applicable for any Hamiltonian function;
- have the Lie–Poisson properties intrinsically encoded.

### 3.3.1 Constrained Hamiltonian systems

Here, we discuss various approaches to construct structure preserving integrators for *constrained* Hamiltonian systems, i.e. Hamiltonian systems on manifolds. The main difference compared to Hamiltonian systems on  $\mathbb{R}^{2d}$  is that now we require not only symplecticity from the numerical flow, but also the flow to be confined to a manifold.

An important example of constrained Hamiltonian systems is Poisson systems, and, in particular, Lie–Poisson systems, that play an important role in classical mechanics and mathematical physics, as it is seen from the previous chapter.

Let  $(q_1, \dots, q_d) \in \mathbb{R}^d$  be the position coordinates. Assume that the dynamics of a mechanical system evolves not on the entire  $\mathbb{R}^d$  but on its submanifold given by *constraints*

$$\mathbb{R}^d \supset Q = \{g(q) = 0\} = \{g_1(q) = 0, \dots, g_m(q) = 0\},$$

where  $m < d$  is the number of constraints, and therefore the dimension of  $Q$  is  $\dim(Q) = d - m$ .

The Hamiltonian function is adjusted by adding the Lagrange multipliers  $(\lambda_1, \dots, \lambda_m)$ :

$$\tilde{H}(p, q, \lambda) = H(p, q) + g(q)^T \lambda,$$

and Hamilton's equations in this case are

$$\dot{q} = H_p(p, q), \quad \dot{p} = -H_q(p, q) - G(q)^T \lambda, \quad g(q) = 0, \quad (3.8)$$

where

$$G(q) = \frac{\partial(g_1, \dots, g_m)}{\partial(q_1, \dots, q_d)}$$

is the Jacobian of  $g(q)$ .

**Example 3.1** (Spherical pendulum). Consider a mechanical system that consists of a point mass  $m$  on a massless rod of the length  $l$  that can rotate around a fixed point  $O \in \mathbb{R}^3$  in the presence of the gravitational field. The Hamiltonian of such system is

$$H(p, q) = T + U = \frac{p_1^2 + p_2^2 + p_3^2}{2m} + mgq_3,$$

where  $g$  is the free-fall acceleration, and the dynamics is evolving on the sphere given by the constraint

$$0 = g(q) = q_1^2 + q_2^2 + q_3^2 - l^2.$$

Let us obtain the expression for  $\lambda(p, q)$ , which we will later plug into (3.8). This process is called an *index reduction*. To that end, let us differentiate the constraint  $g(q) = 0$  with respect to time subject to (3.8). We get

$$0 = \frac{d}{dt}(g(q(t))) = G(q)\dot{q} = G(q)H_p(p, q).$$

Differentiating second time, we get

$$0 = \frac{\partial}{\partial q}(G(q)H_p)H_p + GH_{pp}H_q + GH_{pp}G^T\lambda.$$

Assuming that the matrix  $GH_{pp}G^T$  is invertible, one can express  $\lambda = \lambda(p, q)$ . Inserting  $\lambda(p, q)$  into (3.8), we get

$$\dot{q} = H_p(p, q), \quad \dot{p} = -H_q(p, q) - G(q)^T\lambda(p, q), \quad (3.9)$$

which is a Hamiltonian system on the cotangent bundle of  $Q$ :

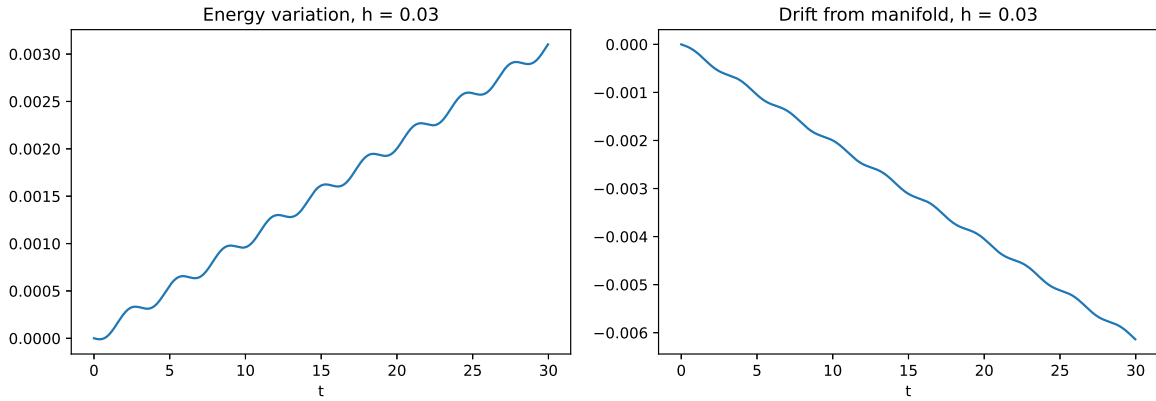
$$M = T^*Q = \{(p, q) \in T^*\mathbb{R}^d \simeq \mathbb{R}^{2d} \mid g(q) = 0, G(q)H_p(p, q) = 0\}$$

It is worth mentioning that equations (3.9) no longer have a structure of canonical equations on  $\mathbb{R}^{2d}$ , because of the presence of the term with  $\lambda(p, q)$ . However, we can still apply the symplectic Euler method to (3.9).

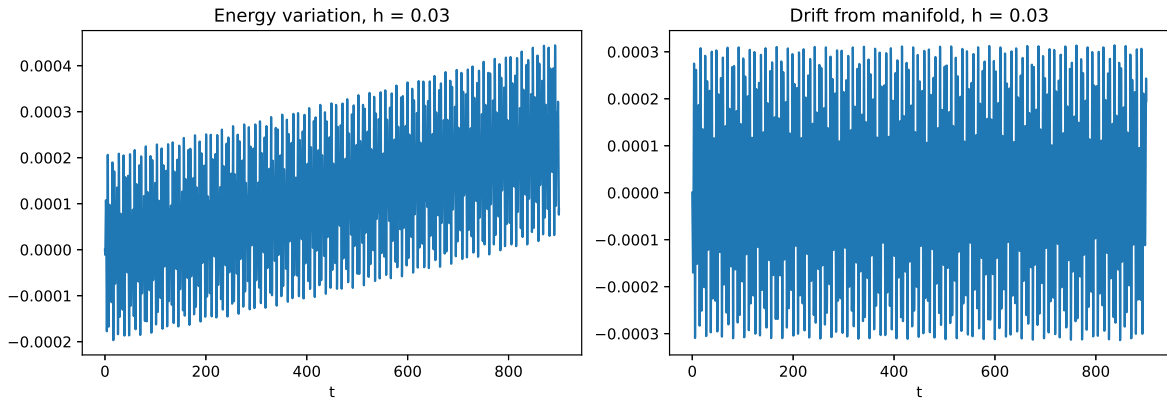
One can see from Fig. 3.3 that the symplectic Euler method implemented without projection to  $Q$  does not preserve the energy of the system. Also, numerical flow is drifting away from the manifold.

If we use the projection to  $Q$ , i.e. replace the combination  $q_1^2 + q_2^2 + q_3^2$  in the method with  $l^2$ , we still observe the energy drift (much smaller values on much larger time scale), but the method is nearly staying on the manifold  $Q$ , see Fig. 3.4.

From the simulations, one can conclude that the index reduction is not compatible with symplecticity.



**Fig. 3.3.** Energy drift (left) and drift from the manifold (right). Symplectic Euler method (no projection) does not preserve energy and is not constrained to the manifold.



**Fig. 3.4.** Energy drift (left) and drift from the manifold (right). Symplectic Euler method (with projection) does not preserve energy, but nearly preserves the manifold.

### Symplectic first order method

Here, we will not follow the index reduction process. Instead, we will discretize the system

$$\dot{q} = H_p(p, q), \quad \dot{p} = -H_q(p, q) - G(q)^T \lambda$$

along with constraints

$$g(q) = 0, \quad G(q)H_p(p, q) = 0$$

first by an implicit in  $p$  and explicit in  $q$  step

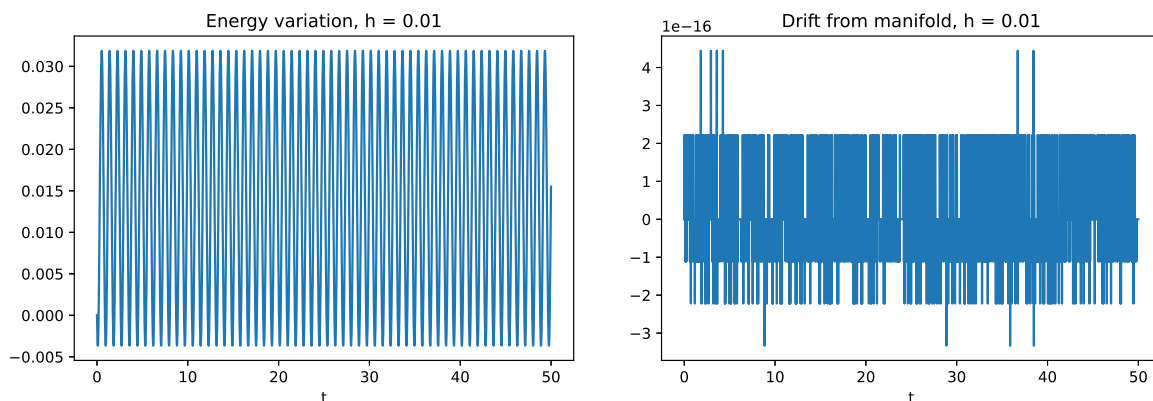
$$\begin{aligned} \hat{p} &= p_n - h(H_q(\hat{p}, q_n) + G(q_n)^T \lambda_{n+1}), \\ q_{n+1} &= q_n + hH_p(\hat{p}, q_n), \\ 0 &= g(q_{n+1}) \end{aligned} \tag{3.10}$$

with unknowns  $\hat{p}$ ,  $q_{n+1}$ ,  $\lambda_{n+1}$ . This already implies that  $q_{n+1} \in Q$ . Now, using projection we force the variable  $p$  to be in  $T_q^*Q$ :

$$\begin{aligned} p_{n+1} &= \hat{p} - hG(q_{n+1})^T \mu_{n+1}, \\ 0 &= G(q_{n+1})H_p(p_{n+1}, q_{n+1}), \end{aligned} \quad (3.11)$$

with unknowns  $p_{n+1}$ ,  $\mu_{n+1}$ .

The method (3.10)–(3.11) is symplectic and has convergence order 1. Simulation results in Fig. 3.5 show that the method nearly preserves the energy and exactly preserves the manifold.



**Fig. 3.5.** Energy drift (left) and drift from the manifold (right).

## SHAKE and RATTLE

The methods SHAKE and RATTLE, originally developed for molecular dynamics, are of second order and are symmetric and symplectic.

Consider a separable Hamiltonian

$$H(p, q) = \frac{1}{2}p^T M^{-1}p + U(q),$$

with constant mass matrix  $M$ . The corresponding Newton equation is

$$M\ddot{q} = -U_q(q) - G(q)^T \lambda, \quad g(q) = 0. \quad (3.12)$$

## SHAKE

A straightforward extension of the Störmer–Verlet scheme gives the following discretization for (3.12), called SHAKE:

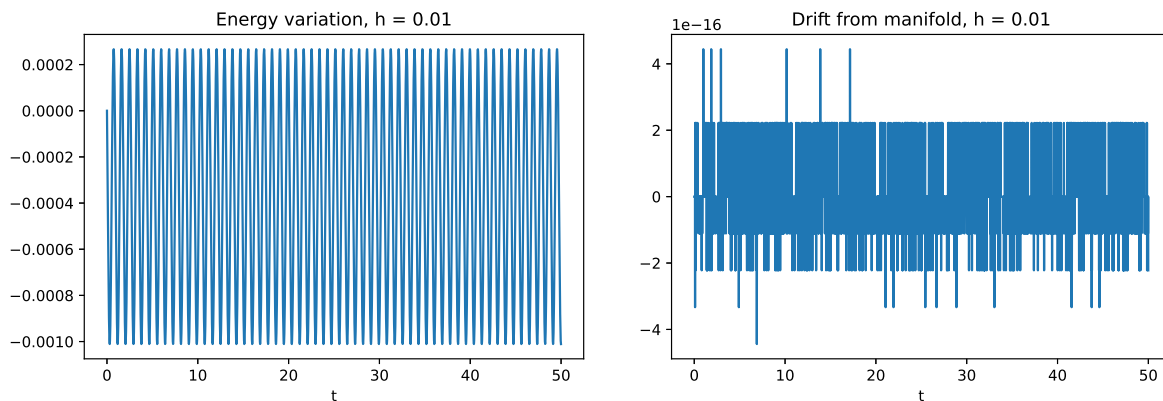
$$\begin{aligned} q_{n+1} - 2q_n + q_{n-1} &= -h^2 M^{-1}(U(q_n) + G(q_n)^T \lambda_n), \\ 0 &= g(q_{n+1}). \end{aligned} \quad (3.13)$$

## RATTLE

Formulation of SHAKE as in (3.13) may lead to accumulation of round-off errors. Its modification to a one-step method called RATTLE is formulated for general Hamiltonians as follows:

$$\begin{aligned}
 \widehat{p} &= p_n - \frac{h}{2}(H_q(\widehat{p}, q_n) + G(q_n)^T \lambda_n), \\
 q_{n+1} &= q_n + \frac{h}{2}(H_p(\widehat{p}, q_n) + H_p(\widehat{p}, q_{n+1})), \\
 0 &= g(q_{n+1}), \\
 p_{n+1} &= \widehat{p} - \frac{h}{2}(H_q(\widehat{p}, q_{n+1}) + G(q_{n+1})^T \mu_n), \\
 0 &= G(q_{n+1})H_p(p_{n+1}, q_{n+1}).
 \end{aligned} \tag{3.14}$$

Simulation results shown in Fig. 3.6 show that the method nearly preserves the Hamiltonian with variations of magnitude  $\sim 10^{-4}$  (compared to  $\sim 10^{-2}$  for the symplectic method from the previous section), and also exactly preserves the manifold.



**Fig. 3.6.** Energy drift (left) and drift from the manifold (right).

### 3.3.2 Poisson systems as constrained Hamiltonian systems

Let  $F$  and  $G$  be smooth functions on a smooth manifold  $M$  with local coordinates  $y = (y_1, \dots, y_n)$ . Let us define a bilinear operation on the space of smooth functions on  $M$  as follows:

$$\{F, G\} = \sum_{i,j=1}^n \frac{\partial F}{\partial y_i} b_{ij}(y) \frac{\partial G}{\partial y_j} = (\nabla F)^T B(y) \nabla G, \tag{3.15}$$

where  $B = (b_{ij}(y))$  is a smooth matrix-valued function called *structure matrix*. If the matrix  $B$  has the following properties

- Skew-symmetry:  $b_{ij} = -b_{ji}$
- Fulfils the identity

$$\sum_{l=1}^n \left( \frac{\partial b_{ij}}{\partial y_l} b_{lk} + \text{cycle over } (i, j, k) \right) = 0,$$

then the bracket (3.15) becomes a *Poisson bracket*.

The corresponding equations

$$\dot{y} = B(y)\nabla H(y) \tag{3.16}$$

for some function  $H(y)$ , are called *Poisson equations*.

**Example 3.2.** 1. If  $B = J^{-1}$ , where

$$J = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix},$$

then  $\dot{y} = J^{-1}\nabla H$  — these are the canonical Hamilton's equations.

2. If  $b_{ij}(y) = \sum_{k=1}^n c_{ij}^k y_k$ , then the corresponding equations (3.16) are called *Lie–Poisson equations*.

There are special types of conserved quantities  $C(y)$  of (3.16) that are first integrals of (3.16) for any choice of the Hamiltonian function. They are called *Casimirs* and satisfy

$$\nabla C(y)^T B(y) = 0.$$

It turns out that any constrained Hamiltonian system can be seen as a Poisson system. Indeed, let us rewrite equations (3.8) as follows:

$$\dot{x} = J^{-1} \left( \nabla H + \sum_{i=1}^m \lambda_i(x) \nabla g_i(x) \right) \tag{3.17}$$

with  $x = (p, q) \in M$ , where the manifold  $M$  is defined as

$$M = \{x \mid c(x) = 0\}$$

with  $c(x) = (g(q), G(q)H_p(p, q))$ .

Let  $y \in \mathbb{R}^{2(d-m)} \simeq M$  be the local coordinates on  $M$ , so that  $x = \chi(y)$ . Rewriting (3.17) in terms of new coordinates  $y$  we obtain

$$X(y)\dot{y} = J^{-1} \left( \nabla_x H(\chi(y)) + \sum_{i=1}^m \lambda_i(\chi(y)) \nabla g_i(\chi(y)) \right),$$

where  $X(y) = \partial\chi/\partial y$  is the Jacobian of  $\chi(y)$ . Multiplication by  $X(y)^T J$  from the left allows one to get rid of the contribution with Lagrange multipliers, and we finally get the Poisson form of (3.17):

$$\dot{y} = \underbrace{(X(y)^T J X(y))^{-1}}_{B(y)} \underbrace{X(y)^T \nabla_x H(\chi(y))}_{\nabla_y K(y)},$$

where  $K(y) = H(\chi(y))$ .

This important observation, that constrained Hamiltonian systems can be treated as Poisson systems, can be seen the other way around as well: having a Poisson system one can relate it to some constrained Hamiltonian system. This drives to the idea of constructing Poisson integrators for Poisson systems out of corresponding integrators for constrained Hamiltonian systems.

But let us first clarify what we mean exactly by a Poisson integrator. To that end, let us list the main properties of the flow  $\varphi_t(y)$  of a Poisson system.

- $\varphi_t(y)$  is a Poisson map, i.e.

$$\varphi'_t(y) B(y) \varphi'_t(y)^T = B(\varphi_t(y)).$$

In particular, for  $B = J^{-1}$  it reduces to the symplecticity of a canonical Hamiltonian flow.

- $\varphi_t(y)$  respects the Casimirs, i.e.  $C(\varphi_t(y)) = \text{const}$ .

In light of the above properties of  $\varphi_t(y)$  it is natural to say that a numerical method  $y_1 = \Phi_h(y_0)$  is said to be a *Poisson integrator*, if  $\Phi_h$  is a Poisson map and if it preserves the coadjoint orbits (and therefore, the Casimirs).

The following Lemma based on the above mentioned relation between constrained Hamiltonian and Poisson systems provides a strategy of finding a Poisson integrator.

**Lemma 3.1.** *An integrator  $x_1 = \Psi_h(x_0)$  for a Hamiltonian system on  $M$  is symplectic if and only if the integrator  $y_1 = \Phi_h(y_0)$  is a Poisson integrator.*

**Example 3.3** (Rigid body). As an example of a Poisson system (in fact, Lie–Poisson) we will consider the rigid body dynamics, which is given by the Poisson equations (3.16) with  $y = (y_1, y_2, y_3)^T$  representing the angular momentum,

$$B(y) = \begin{pmatrix} 0 & -y_3 & y_2 \\ y_3 & 0 & -y_1 \\ -y_2 & y_1 & 0 \end{pmatrix}, \quad H(y) = \frac{1}{2} \sum_{k=1}^3 \frac{y_k^2}{I_k},$$

where  $I_1, I_2, I_3$  are moments of inertia.

We see that the entries of the matrix  $B(y)$  are linear functions in  $y_i$ , and therefore the rigid body dynamics is an example of a Lie–Poisson system.

The corresponding constrained Hamiltonian system is

$$\begin{cases} \dot{Q} = PD^{-1}, \\ \dot{P} = -Q\Lambda, \\ 0 = Q^T Q - I, \end{cases} \quad (3.18)$$

where  $D = \text{diag}(d_1, d_2, d_3)$  with

$$I_1 = d_2 + d_3, \quad I_2 = d_3 + d_1, \quad I_3 = d_1 + d_2,$$

$\Lambda$  is a symmetric matrix representing Lagrange multipliers, and the vector  $y = (y_1, y_2, y_3)$  is reconstructed from  $(P, Q)$  via the matrix  $Y = Q^T P$  as follows:

$$\begin{pmatrix} 0 & -y_3 & y_2 \\ y_3 & 0 & -y_1 \\ -y_2 & y_1 & 0 \end{pmatrix} = 2 \text{skew}(Y) = Y - Y^T.$$

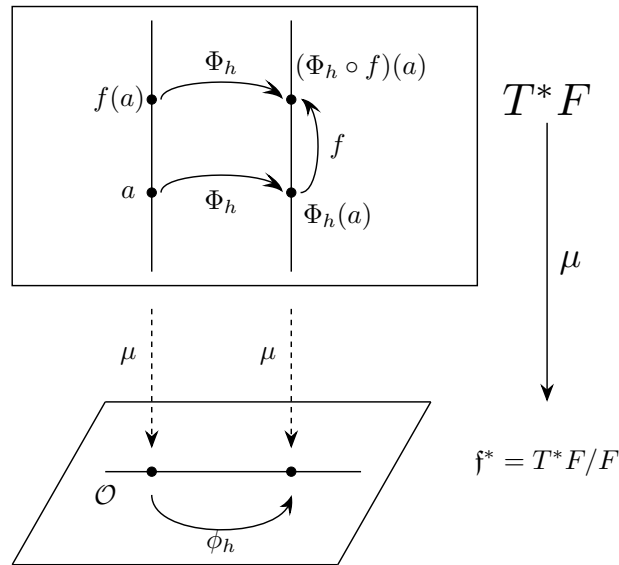
Let us apply RATTLE to (3.18). This results in the following method  $(P_0, Q_0) \mapsto (P_1, Q_1)$  for integrating the rigid body equations:

$$\begin{cases} P_{1/2} = P_0 - \frac{h}{2} Q_0 \Lambda_0, \\ Q_1 = Q_0 + h P_{1/2} D^{-1}, \quad Q_1^T Q_1 = I, \\ P_1 = P_{1/2} - \frac{h}{2} Q_1 \Lambda_1, \quad Q_1^T P_1 D^{-1} + D^{-1} P_1^T Q_1 = 0. \end{cases}$$

### 3.3.3 Discrete Lie–Poisson reduction

In Sect. 2.2.2, we showed that Hamiltonian systems on  $T^*F$  invariant with respect to the lifted cotangent action of  $F$  on  $T^*F$  can be reduced to Lie–Poisson flows on  $\mathfrak{f}^*$  confined to a coadjoint orbit  $\mathcal{O}$ . As any symmetry reduction, this allows to work with systems of smaller dimension and thus simplifies the analysis. From the perspective of geometric integrators, however, the inverse process of Lie–Poisson reconstruction is more important. Indeed, the problem of discretizing Poisson flows is more delicate than that of canonical Hamiltonian systems, so a natural question arises: can one find a correspondence between a given Poisson system and some canonical Hamiltonian system? For general Poisson flows, we have shown the possibility to relate them to constrained Hamiltonian systems (hence reducing the problem to the already solved one). In light of the Lie–Poisson reduction, the natural canonical Hamiltonian system for a Lie–Poisson equation on  $\mathfrak{f}^*$  is the reconstructed right (left) invariant Hamiltonian system on  $T^*F$ . Then, one can apply a symplectic integrator for this Hamiltonian system, and using the Lie–Poisson reduction map it back to  $\mathfrak{f}^*$ , see Fig. 3.7.

Since the Lie–Poisson reduction works for right (left) invariant symplectic maps, the symplectic integrator must also fulfill the *equivariance property*, i.e.



**Fig. 3.7.** Discrete Lie–Poisson reduction (figure taken from Paper I). Symplectic equivariant method  $\Phi_h: T^*F \rightarrow T^*F$  descends to a Lie–Poisson method  $\phi_h: \mathfrak{f}^* \rightarrow \mathfrak{f}^*$ .

commutation with the  $F$ -action on  $T^*F$ . Summarizing, we can formulate the following theorem that allows to construct Lie–Poisson integrators for Lie–Poisson systems out of symplectic integrators for Hamiltonian systems:

**Theorem 3.2.** *If  $\Phi_h: T^*F \rightarrow T^*F$  is a symplectic left (right)-invariant integrator, then its reduction  $\phi_h: \mathfrak{f}^* \rightarrow \mathfrak{f}^*$  is a Lie–Poisson integrator.*



## 4 Finite-mode approximations for 2D fluids

The motion of two-dimensional ideal (magnetized) fluids is governed by the equations with infinite number of conserved quantities called *Casimirs*. The dynamics is confined to the coadjoint orbits, where the Casimirs are constant, endowed with a symplectic structure, and the corresponding flows (governed by the Euler or MHD equations) are symplectic diffeomorphisms of these orbits. This rich geometric structure of phase space motivates the development of finite-dimensional approximations consistent with the aforementioned geometry. Such finite-mode truncations were produced by V. Zeitlin on the flat torus  $\mathbb{T}^2$  in the works [48, 50] and are referred to as *sine-bracket truncations*, and on the sphere  $S^2$  in [49]. In this chapter, we review the key concepts that stand behind these discretizations.

### 4.1 Geometry of 2D magnetized fluids

The system of MHD equations (2.46) discussed previously admits a *vorticity formulation* on simply connected two-dimensional domains  $M$ :

$$\begin{cases} \dot{\omega} = \{\omega, \psi\} + \{\theta, j\}, & \omega = \Delta\psi, \\ \dot{\theta} = \{\theta, \psi\}, & j = \Delta\theta, \end{cases} \quad (4.1)$$

where  $\{\cdot, \cdot\}$  is the Poisson bracket on  $M$ , and  $\omega$  is the vorticity,  $\psi$  is the stream function,  $\theta$  is the magnetic potential, and  $j$  is the current density. From the Stokes theorem, it follows that  $\int_M \omega = 0$ , and without loss of generality, one can assume also  $\int_M \psi = 0$ .

The system (4.1) can be written in the Hamiltonian form

$$\dot{F} = \llbracket F, H \rrbracket,$$

where  $F$  is an observable of the fields  $\omega$  and  $\theta$ , where  $\llbracket \cdot, \cdot \rrbracket$  is the *semidirect product Lie–Poisson bracket* (see [20, 22, 38]):

$$\llbracket F, G \rrbracket = \int_M \left[ \omega \left\{ \frac{\delta F}{\delta \omega}, \frac{\delta G}{\delta \omega} \right\} + \theta \left( \left\{ \frac{\delta F}{\delta \theta}, \frac{\delta G}{\delta \omega} \right\} + \left\{ \frac{\delta F}{\delta \omega}, \frac{\delta G}{\delta \theta} \right\} \right) \right] \mu, \quad (4.2)$$

and  $H(\omega, \theta)$  is the Hamiltonian:

$$H = \frac{1}{2} \int_M (|\nabla\psi|^2 + |\nabla\theta|^2) \mu = -\frac{1}{2} \int_M (\omega\psi + \theta j) \mu. \quad (4.3)$$

A direct computation shows that the following quantities are Casimirs for (4.2):

$$\mathcal{C}_f = \int_M f(\theta) \mu, \quad \mathcal{I}_g = \int_M \omega g(\theta) \mu, \quad (4.4)$$

for arbitrary smooth functions  $f: \mathbb{R} \rightarrow \mathbb{R}$  and  $g: \mathbb{R} \rightarrow \mathbb{R}$ , i.e.,  $[[\mathcal{C}_f, \mathcal{J}]] = [[\mathcal{I}_g, \mathcal{J}]] = 0$  for any functional  $\mathcal{J}$ .

In the case of the trivial magnetic field,  $\theta = 0$ , system (4.1) reduces to

$$\dot{\omega} = \{\omega, \psi\}, \quad \omega = \Delta\psi, \quad (4.5)$$

which is the vorticity formulation of the incompressible Euler equation on  $M$ , and the Lie–Poisson bracket (4.2) becomes

$$[[F, G]] = \int_M \omega \left\{ \frac{\delta F}{\delta \omega}, \frac{\delta G}{\delta \omega} \right\} \mu, \quad (4.6)$$

and the Hamiltonian becomes

$$H = -\frac{1}{2} \int_M (\omega\psi) \mu, \quad (4.7)$$

and the Casimirs become

$$\mathcal{C}_m = \int_M \omega^m \mu, \quad m = 1, 2, \dots, \quad (4.8)$$

where we have made the choice of an arbitrary function  $f$  to be the monomials.

The Hamiltonian structures underlying the equations of ideal (magneto)-hydrodynamics imply the existence of an infinite collection of conserved quantities. This rises a natural question: is there a discrete approximation of equations (4.1) and (4.5) consistent with the aforementioned structures?

In what follows, we discuss the concepts of finite-mode approximations for the Euler equation (4.5) and the Lie–Poisson structure (4.6). Once these concepts are understood for the Euler equations, further generalizations for MHD are discussed.

## 4.2 Zeitlin’s equations on $\mathbb{T}^2$

### 4.2.1 Euler’s equations in the Fourier space

We start with the discussion of the so-called naive truncations of the Euler equations (4.5) on the flat torus  $\mathbb{T}^2 = S^1 \times S^1$  (doubly periodic rectangle). Let

$\mathbf{m} = (m_1, m_2) \in \mathbb{Z}^2$ ,  $\mathbb{Z}_0^2 = \mathbb{Z}^2 \setminus (0, 0)$  and  $\mathbf{x} = (x_1, x_2) \in \mathbb{T}^2$ . Then, decomposing the fields  $\omega$  and  $\psi$  in the basis  $\exp(i(\mathbf{m} \cdot \mathbf{x}))$  as

$$\begin{aligned}\omega(t, \mathbf{x}) &= \sum_{\mathbf{m} \in \mathbb{Z}_0^2} \omega_{\mathbf{m}}(t) \exp(i(\mathbf{m} \cdot \mathbf{x})), \\ \psi(t, \mathbf{x}) &= - \sum_{\mathbf{m} \in \mathbb{Z}_0^2} \frac{\omega_{\mathbf{m}}(t)}{|\mathbf{m}|^2} \exp(i(\mathbf{m} \cdot \mathbf{x})),\end{aligned}\tag{4.9}$$

and inserting them into (4.5), we get the following dynamical system for the Fourier coefficients  $\omega_{\mathbf{m}}(t)$ :

$$\dot{\omega}_{\mathbf{m}} = \sum_{\mathbf{k} \in \mathbb{Z}_0^2} |\mathbf{k}|^{-2} (\mathbf{k} \times \mathbf{m}) \omega_{\mathbf{k}+\mathbf{m}} \omega_{-\mathbf{k}},\tag{4.10}$$

where  $\mathbf{k} \times \mathbf{m} = k_1 m_2 - k_2 m_1$ .

*Remark 4.1.* Summation in (4.9) is done over all the modes except the origin, because the corresponding Fourier coefficient  $\omega_{00} = 0$ , which follows from  $\int_{\mathbb{T}^2} \omega = 0$ .

Doing the same with the Hamiltonian yields

$$H = \frac{1}{2} \sum_{\mathbf{k} \in \mathbb{Z}_0^2} \frac{\omega_{\mathbf{k}} \omega_{-\mathbf{k}}}{\mathbf{k}^2}.\tag{4.11}$$

For the Casimirs (4.8), the computations are less obvious, so we formulate it as a proposition.

**Proposition 4.1.** *The Casimirs (4.8) take the following form in the Fourier space:*

$$\mathcal{C}_{\mathcal{N}} = \sum_{\mathbf{m}_1 + \dots + \mathbf{m}_{\mathcal{N}} = 0} \omega_{\mathbf{m}_1} \omega_{\mathbf{m}_2} \dots \omega_{\mathbf{m}_{\mathcal{N}}}, \quad \mathcal{N} = 1, 2, \dots\tag{4.12}$$

*Proof.* Inserting (4.9) into (4.8), we get

$$\begin{aligned}& \int_{\mathbb{T}^2} \left( \sum_{\mathbf{m}_1} \omega_{\mathbf{m}_1} \exp(i(\mathbf{m}_1 \cdot \mathbf{x})) \right) \dots \left( \sum_{\mathbf{m}_{\mathcal{N}}} \omega_{\mathbf{m}_{\mathcal{N}}} \exp(i(\mathbf{m}_{\mathcal{N}} \cdot \mathbf{x})) \right) d\mathbf{x} = \\ & \int_{\mathbb{T}^2} \sum_{\mathbf{m}_1, \mathbf{m}_2, \dots, \mathbf{m}_{\mathcal{N}}} \omega_{\mathbf{m}_1} \omega_{\mathbf{m}_2} \dots \omega_{\mathbf{m}_{\mathcal{N}}} \exp \left( i \left( \sum_{j=1}^{\mathcal{N}} \mathbf{m}_j \right) \cdot \mathbf{x} \right) d\mathbf{x}.\end{aligned}$$

Since the functions  $\exp(i(\mathbf{m} \cdot \mathbf{x}))$  integrate to zero over  $\mathbb{T}^2$  if  $\mathbf{m} \neq (0, 0)$ , then the only non-trivial contributions to the sum will come from the terms with  $\sum_{j=1}^{\mathcal{N}} \mathbf{m}_j = 0$ , which implies the assertion.  $\square$

The next step is to get the expression for the fluid bracket (4.6).

**Proposition 4.2.** *The fluid bracket (4.6) in the Fourier space takes the following form:*

$$\llbracket F, G \rrbracket = 4\pi^2 \sum_{\mathbf{k}, \mathbf{m} \in \mathbb{Z}^2} \omega_{\mathbf{k}+\mathbf{m}} (\mathbf{k} \times \mathbf{m}) \frac{\partial F}{\partial \omega_{\mathbf{m}}} \frac{\partial G}{\partial \omega_{\mathbf{k}}}, \quad (4.13)$$

for  $F = F(\omega_{\mathbf{m}})$ ,  $G = G(\omega_{\mathbf{m}})$ ,  $\mathbf{m} \in \mathbb{Z}^2$ .

*Proof.* Let us take two functionals  $F(\omega)$  and  $G(\omega)$ . One can view these functions as those depending on the Fourier coefficients, i.e.  $F(\omega) = F(\sum_{\mathbf{m}} \omega_{\mathbf{m}} e^{i(\mathbf{m} \cdot \mathbf{x})}) = \tilde{F}(\omega_{\mathbf{m}})$ . Using the inverse Fourier transform

$$\omega_{\mathbf{m}} = \int_{\mathbb{T}^2} \omega \exp(-i(\mathbf{m} \cdot \mathbf{x})) d\mathbf{x},$$

and the chain rule

$$\frac{\delta F}{\delta \omega} = \sum_{\mathbf{m} \in \mathbb{Z}^2} \frac{\partial \tilde{F}}{\partial \omega_{\mathbf{m}}} \frac{\delta \omega_{\mathbf{m}}}{\delta \omega} = \sum_{\mathbf{m} \in \mathbb{Z}^2} \frac{\partial \tilde{F}}{\partial \omega_{\mathbf{m}}} \exp(-i(\mathbf{m} \cdot \mathbf{x})),$$

we get

$$\begin{aligned} \llbracket F, G \rrbracket &= \int_{\mathbb{T}^2} \left( \sum_{\mathbf{m}' \in \mathbb{Z}^2} \omega_{\mathbf{m}'} \exp(-i(\mathbf{m}' \cdot \mathbf{x})) \right) \sum_{\mathbf{m} \in \mathbb{Z}^2} \sum_{\mathbf{k} \in \mathbb{Z}^2} \frac{\partial \tilde{F}}{\partial \omega_{\mathbf{m}}} \frac{\partial \tilde{G}}{\partial \omega_{\mathbf{k}}} \times \\ &\quad \{ \exp(-i(\mathbf{m} \cdot \mathbf{x})), \exp(-i(\mathbf{k} \cdot \mathbf{x})) \} d\mathbf{x}. \end{aligned} \quad (4.14)$$

For the Poisson bracket of the exponential functions, we get

$$\{ \exp(-i(\mathbf{m} \cdot \mathbf{x})), \exp(-i(\mathbf{k} \cdot \mathbf{x})) \} = (\mathbf{k} \times \mathbf{m}) \exp(-i((\mathbf{k} + \mathbf{m}) \cdot \mathbf{x})).$$

Hence, (4.14) becomes

$$\begin{aligned} \llbracket F, G \rrbracket &= \sum_{\mathbf{m}', \mathbf{m}, \mathbf{k} \in \mathbb{Z}^2} \omega_{\mathbf{m}'} \frac{\partial \tilde{F}}{\partial \omega_{\mathbf{m}}} \frac{\partial \tilde{G}}{\partial \omega_{\mathbf{k}}} (\mathbf{k} \times \mathbf{m}) \underbrace{\int_{\mathbb{T}^2} \exp(i((\mathbf{m}' - \mathbf{k} - \mathbf{m}) \cdot \mathbf{x})) d\mathbf{x}}_{4\pi^2 \delta(\mathbf{m}' - \mathbf{k} - \mathbf{m})} = \\ &= \sum_{\mathbf{m}, \mathbf{k} \in \mathbb{Z}^2} 4\pi^2 \omega_{\mathbf{k}+\mathbf{m}} (\mathbf{k} \times \mathbf{m}) \frac{\partial \tilde{F}}{\partial \omega_{\mathbf{m}}} \frac{\partial \tilde{G}}{\partial \omega_{\mathbf{k}}} = \llbracket \tilde{F}, \tilde{G} \rrbracket. \end{aligned}$$

□

Summarizing, we have now obtained all the key ingredients of the Hamiltonian formulation of the Euler equations (4.5) in the Fourier space: the equations themselves (4.10), the Hamiltonian (4.11), the Casimirs (4.12), and the Lie–Poisson structure (4.13). Let us now give the Euler–Arnold interpretation of (4.10).

We start with an abstract Lie algebra  $\mathcal{L}$ , i.e., a vector space with a Lie bracket  $[\cdot, \cdot]$ . The first key ingredient of a general Euler–Arnold equation is the Lie algebra

structure. If  $L_1, L_2, \dots$  is a basis in  $\mathcal{L}$ , then the *structure constants*  $C_{ij}^k$  of  $\mathcal{L}$  are defined as

$$[L_i, L_j] = \sum_k C_{ij}^k L_k.$$

Let now  $\mathcal{L}^*$  be its dual. Then, one can introduce a Lie–Poisson structure

$$\llbracket f, g \rrbracket = \sum_{i,j,k} C_{ij}^k \omega_k \frac{\delta f}{\delta \omega_i} \frac{\delta g}{\delta \omega_j}, \quad f, g \in C^\infty(\mathcal{L}^*). \quad (4.15)$$

The second key ingredient is the inertia operator  $I: \mathcal{L} \rightarrow \mathcal{L}^*$  usually provided by the metric tensor  $g^{lj}$  and defining the energy

$$H = \frac{1}{2} \sum_{i,j} g^{ij} \omega_i \omega_j.$$

And finally, the Euler–Arnold equations on  $\mathcal{L}^*$  take the form:

$$\dot{\omega}_i = \sum_{j,k,l} g^{lj} C_{ij}^k \omega_l \omega_k. \quad (4.16)$$

One can check that  $\dot{H} = 0$  along the trajectories of (4.16).

Let now  $\mathcal{L}$  be the algebra of smooth functions on  $\mathbb{T}^2$ . The basis is given by  $\phi_{\mathbf{n}} = \exp(i(\mathbf{n} \cdot \mathbf{x}))$ . The structure constants are obtained by taking the Poisson bracket of the basis functions:

$$[\phi_{\mathbf{n}}, \phi_{\mathbf{m}}] = (\mathbf{m} \times \mathbf{n}) \phi_{\mathbf{n}+\mathbf{m}} = \sum_{\mathbf{k} \in \mathbb{Z}^2} C_{\mathbf{nm}}^{\mathbf{k}} \phi_{\mathbf{k}}, \quad (4.17)$$

with the structure constants

$$C_{\mathbf{nm}}^{\mathbf{k}} = (\mathbf{m} \times \mathbf{n}) \delta(\mathbf{k} - \mathbf{n} - \mathbf{m}). \quad (4.18)$$

To make a connection between (4.16) and (4.10), we need to choose the metric tensor as follows:

$$g^{\mathbf{kl}} = \delta(\mathbf{k} + \mathbf{l}) |\mathbf{k}|^{-2}. \quad (4.19)$$

We thus arrive at the following result.

**Theorem 4.1.** *The Euler equations in the Fourier space (4.10) have the form of the Euler–Arnold equation (4.16), with the structure constants (4.18) and the metric (4.19). In terms of the Lie–Poisson bracket in the Fourier space (4.13), they take the form  $\dot{\omega}_{\mathbf{m}} = \llbracket \omega_{\mathbf{m}}, H \rrbracket$ , with the Hamiltonian (4.11) preserved by the flow (4.10). The quantities (4.12) are Casimirs of the bracket (4.13).*

One can perform the naive truncation of equations (4.10) by simply running the frequencies  $\mathbf{k}$  and  $\mathbf{m}$  over a box  $\mathbf{k}, \mathbf{m} \in ([-N, N] \times [-N, N]) \setminus (0, 0) = \mathcal{B}$  rather than over  $\mathbb{Z}^2$ . This results in  $(2N + 1)^2$  dimensional dynamical system:

$$\dot{\omega}_{\mathbf{m}} = \sum_{\mathbf{k} \in \mathcal{B}} |\mathbf{k}|^{-2} (\mathbf{k} \times \mathbf{m}) \omega_{\mathbf{k}+\mathbf{m}} \omega_{-\mathbf{k}}, \quad \mathbf{m} \in \mathcal{B}. \quad (4.20)$$

Equations (4.20) are problematic in several aspects:

1. equations (4.20) are not Hamiltonian, as the truncation of the bracket (4.13) fails to fulfill the Jacobi identity,
2. the Casimirs (4.12) are not preserved, except for  $\mathcal{C}_2$ ,
3. some of the variables  $\omega_{\mathbf{k}+\mathbf{m}}$  are outside of the summation box  $\mathcal{B}$ .

### 4.2.2 Sine-bracket approximation for the Euler equations

The *sine-bracket approximation* is a way to overcome the mentioned difficulties of equations (4.20) and to construct a self-consistent truncated analog of the Euler (and MHD) equations, which is itself an Euler–Arnold equation on the dual of a suitable Lie algebra. The key idea behind the sine-bracket approximation is to truncate the equations (4.10) along with modifying the structure constants (4.18) (and consequently, the Lie–Poisson structure (4.15) on  $\mathcal{L}^*$ ), while keeping the metric tensor (4.19) unchanged. Naturally, in order to recover the Euler equations when sending the truncation parameter  $N \rightarrow \infty$ , the modified structure constants must converge to the original ones. This will result in a new Euler–Arnold equation (4.16) that approximates the original one (4.10).

Let us fix some odd number  $N$  and consider the box  $\mathcal{B}_0 = [-(N-1)/2, (N-1)/2]^2 \setminus (0,0)$ . One observes that since the vorticity field  $\omega(t, \mathbf{x})$  is real-valued, some conditions must be imposed on the complex Fourier coefficients  $\omega_{\mathbf{m}}$ . Indeed,  $\omega(t, \mathbf{x}) = \bar{\omega}(t, \mathbf{x})$  implies  $\omega_{-\mathbf{m}} = \bar{\omega}_{\mathbf{m}}$ , which is the reality condition.

As shown in [13, 12] (see also [5, Ch. I.11] and [48]) commutation relations in the matrix Lie algebras  $\mathfrak{sl}(N, \mathbb{C})$  approximate those in the infinite-dimensional Lie algebra of divergence-free vector fields  $\mathcal{D}_\mu(\mathbb{T}^2)$  realized (in 2D) as the algebra of functions on  $\mathbb{T}^2$ , given by (4.17). Indeed, consider the following two matrices in  $\mathfrak{sl}(N, \mathbb{C})$ :

$$F = \text{diag}(1, \varepsilon, \dots, \varepsilon^{n-1}), \quad H = \begin{pmatrix} 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 1 & \dots & 0 \\ \vdots & \vdots & & \ddots & \\ 0 & 0 & \dots & \dots & 1 \\ 1 & 0 & \dots & \dots & 0 \end{pmatrix},$$

where  $\varepsilon$  is a primitive root of  $N$ -th degree of unity, e.g.  $\varepsilon = e^{i4\pi/N}$ . The matrices  $F$  and  $H$  fulfill the identities  $F^N = H^N = 1$  and  $HF = \varepsilon FH$ .

Define  $(N^2 - 1)$  matrices  $J_{\mathbf{m}}$ ,  $\mathbf{m} = (m_1, m_2) \in \mathcal{B}_0$  by the following way:

$$J_{\mathbf{m}} = \varepsilon^{m_1 m_2 / 2} F^{m_1} H^{m_2}.$$

Then, the matrices  $J_{\mathbf{m}}$  span  $\mathfrak{sl}(N, \mathbb{C})$  and obey the commutation relations

$$[J_{\mathbf{n}}, J_{\mathbf{m}}] = 2i \cdot \sin\left(\frac{2\pi(\mathbf{n} \times \mathbf{m})}{N}\right) J_{\mathbf{n}+\mathbf{m}},$$

as well as  $J_{\mathbf{m}}^\dagger = J_{-\mathbf{m}}$ .

Introducing a new basis  $L_{\mathbf{m}} = (iN/4\pi)J_{\mathbf{m}}$ , we get commutation relations

$$\begin{aligned} [L_{\mathbf{n}}, L_{\mathbf{m}}] &= \frac{N}{2\pi} \sin\left(\frac{2\pi(\mathbf{m} \times \mathbf{n})}{N}\right) L_{\mathbf{m}+\mathbf{n}} \implies \\ C_{\mathbf{nm}}^{\mathbf{k}} &= \frac{N}{2\pi} \sin\left(\frac{2\pi(\mathbf{m} \times \mathbf{n})}{N}\right) \delta(\mathbf{k} - \mathbf{n} - \mathbf{m}), \end{aligned} \quad (4.21)$$

approximating (4.17) and (4.18) respectively, as  $N \rightarrow \infty$ .

Taking the Euler–Arnold equations (4.16) with structure constants (4.21) and metric (4.19), we get the system of equations referred to as *sine-Euler equations*, or *Euler–Zeitlin equations on  $\mathbb{T}^2$* :

$$\dot{\omega}_{\mathbf{m}} = \sum_{\mathbf{k} \in \mathcal{B}_0} |\mathbf{k}|^{-2} \frac{N}{2\pi} \sin\left(\frac{2\pi(\mathbf{k} \times \mathbf{m})}{N}\right) \omega_{(\mathbf{k}+\mathbf{m})|_{\text{mod } N}} \omega_{-\mathbf{k}}. \quad (4.22)$$

It is possible to write equations (4.22) in a compact matrix form. Introducing the matrices

$$W = \sum_{\mathbf{m} \in \mathcal{B}_0} \omega_{\mathbf{m}} L_{\mathbf{m}}, \quad P = - \sum_{\mathbf{k} \in \mathcal{B}_0} \omega_{\mathbf{k}} |\mathbf{k}|^{-2} L_{\mathbf{k}}, \quad (4.23)$$

and using the commutation relations (4.21), one can rewrite equations (4.22) as a matrix ODE

$$\dot{W} = [W, P]. \quad (4.24)$$

We further observe that

$$W^\dagger = \sum_{\mathbf{m} \in \mathcal{B}_0} \bar{\omega}_{\mathbf{m}} L_{\mathbf{m}}^\dagger = \sum_{\mathbf{m} \in \mathcal{B}_0} \omega_{-\mathbf{m}} \left(\frac{iN}{4\pi} J_{\mathbf{m}}\right)^\dagger = \sum_{\mathbf{m} \in \mathcal{B}_0} \omega_{-\mathbf{m}} \left(-\frac{iN}{4\pi} J_{-\mathbf{m}}\right) = -W,$$

which implies that  $W \in \mathfrak{su}(N)$ , as well as  $P \in \mathfrak{su}(N)$ . Furthermore, the right hand side of (4.24) coincides with the coadjoint action of  $\mathfrak{su}(N)$  on its dual.

The matrix formulation of the Euler–Zeitlin equations on  $\mathbb{T}^2$  not only resembles the form of the original Euler equations (4.1), but also makes it possible to identify the Casimir invariants as traces of powers of  $W$ , as well as the Hamiltonian function:

$$\mathcal{C}_m^N = \text{tr}(W^m), \quad H^N = -\frac{1}{2} \text{tr}(WP), \quad m = 1, 2, \dots, N. \quad (4.25)$$

*Remark 4.2.* 1. In order for the Casimirs and the Hamiltonian (4.25) to converge to the original counterparts (4.7) and (4.8), as  $N \rightarrow \infty$ , one needs an appropriate multiplier depending on  $N$  in front of (4.25). Here, we omit the discussion about convergence, as it is proved with all necessary details for the case of the sphere in Paper I.

2. Looking at the original fields  $\omega$  and  $\psi$  in (4.9) and at their respective matrix analogues in (4.23), one observes the following correspondence: the basis functions  $\exp(i(\mathbf{m} \cdot \mathbf{x}))$  are formally replaced with the basis matrices  $L_{\mathbf{m}}$ , and the Poisson bracket  $\{\cdot, \cdot\}$  is replaced with the matrix commutator  $[\cdot, \cdot]$ . To this reason, the sine-Euler equations are sometimes called *quantized Euler equations*, following the analogy of transition from classical physics to quantum physics.

We conclude this section with a summary of all the key results about the sine-Euler equations.

**Theorem 4.2.** *The sine-Euler equations (4.22) are a Lie–Poisson flow on the dual of the Lie algebra  $\mathfrak{su}(N)$ , with the Casimir functions and Hamiltonian given by (4.25).*

### 4.2.3 Sine-bracket approximation for MHD

To get the sine-truncation for the MHD equations, one needs the Fourier expansions for the magnetic potential  $\theta(t, \mathbf{x})$  and the current density  $j(t, \mathbf{x})$ , in addition to (4.9):

$$\begin{aligned}\theta(t, \mathbf{x}) &= \sum_{\mathbf{m} \in \mathbb{Z}_0^2} \theta_{\mathbf{m}}(t) \exp(i(\mathbf{m} \cdot \mathbf{x})), \\ j(t, \mathbf{x}) &= - \sum_{\mathbf{m} \in \mathbb{Z}_0^2} \theta_{\mathbf{m}}(t) |\mathbf{m}|^2 \exp(i(\mathbf{m} \cdot \mathbf{x})).\end{aligned}$$

Further, similarly to the Euler equations, we construct two matrices  $\Theta \in \mathfrak{su}(N)$  and  $J \in \mathfrak{su}(N)$  as follows:

$$\Theta = \sum_{\mathbf{m} \in \mathcal{B}_0} \theta_{\mathbf{m}} L_{\mathbf{m}}, \quad J = - \sum_{\mathbf{k} \in \mathcal{B}_0} \theta_{\mathbf{k}} |\mathbf{k}|^2 L_{\mathbf{k}},$$

and the corresponding sine-MHD equations for the modes  $(\omega_{\mathbf{m}}, \theta_{\mathbf{m}})$  take the form

$$\dot{W} = [W, P] + [\Theta, J], \quad \dot{\Theta} = [\Theta, P], \quad W, \Theta, J, P \in \mathfrak{su}(N). \quad (4.26)$$

Equations (4.26) have conservation laws, the Casimirs, given by

$$\mathcal{C}_m^N = \text{tr}(\Theta^m), \quad \mathcal{I}_m^N = \text{tr}(W\Theta^m), \quad m = 1, 2, 3, \dots, N, \quad (4.27)$$

as well as the Hamiltonian

$$H^N = -\frac{1}{2} \text{tr}(WP) - \frac{1}{2} \text{tr}(\Theta J). \quad (4.28)$$

The Lie–Poisson formulation for the sine-MHD equations (4.26) can also be given on the dual of a suitable Lie algebra. This Lie algebra is called the *magnetic extension* of  $\mathfrak{su}(N)$  and is the semidirect product of the algebra itself and its dual. We summarize all the above observations in the following theorem:

**Theorem 4.3.** *The sine-MHD equations (4.26) are a Lie–Poisson flow on the dual  $\mathfrak{f}^*$  of the Lie algebra  $\mathfrak{f} = \mathfrak{su}(N) \ltimes \mathfrak{su}(N)^*$ . The quantities (4.27) are Casimirs for (4.26), and the Hamiltonian (4.28) is conserved by the flow.*

#### 4.2.4 Discrete Laplacian

When constructing the sine-approximations for the Euler equations and MHD, we kept the metric tensor (4.19) from the corresponding Fourier transformed equations on  $\mathbb{Z}^2$ . In general, any tensor that converges to (4.19), as  $N \rightarrow +\infty$ , would be suitable. There is, however, a natural choice of the metric tensor  $g^{\mathbf{kl}}$  coming from the matrix version of the Laplace operator. We observe that the Laplace operator  $\Delta$  is generated from the basis functions and their Poisson brackets:

$$\Delta\phi_{\mathbf{n}} = \frac{1}{2}([\phi_{-1,-1}, [\phi_{1,1}, \phi_{\mathbf{n}}]] + [\phi_{-1,1}, [\phi_{1,-1}, \phi_{\mathbf{n}}]]) = -|\mathbf{n}|^2\phi_{\mathbf{n}}. \quad (4.29)$$

The matrix Laplacian  $\Delta_N: \mathfrak{su}(N) \rightarrow \mathfrak{su}(N)$  can be constructed by replacing the basis functions in (4.29) with the basis matrices  $L_{\mathbf{n}}$ :

$$\begin{aligned} \Delta_N L_{\mathbf{n}} &= \frac{1}{2}([L_{-1,-1}, [L_{1,1}, L_{\mathbf{n}}]] + [L_{-1,1}, [L_{1,-1}, L_{\mathbf{n}}]]) = \\ &= -\frac{1}{2}\left(\frac{N}{2\pi}\right)^2 \left[ \sin^2\left(\frac{2\pi}{N}(n_1 - n_2)\right) + \sin^2\left(\frac{2\pi}{N}(n_1 + n_2)\right) \right] L_{\mathbf{n}}. \end{aligned}$$

Therefore, the choice for the metric tensor  $(g^N)^{\mathbf{nk}}$  could be

$$(g^N)^{\mathbf{nk}} = \delta(\mathbf{n} + \mathbf{k}) \left[ \frac{1}{2}\left(\frac{N}{2\pi}\right)^2 \left[ \sin^2\left(\frac{2\pi}{N}(n_1 - n_2)\right) + \sin^2\left(\frac{2\pi}{N}(n_1 + n_2)\right) \right] \right]^{-1}.$$

Clearly,  $(g^N)^{\mathbf{nk}} \rightarrow g^{\mathbf{nk}}$  in (4.19) as  $N \rightarrow \infty$ .

### 4.3 Zeitlin's equations on $S^2$

In the case of the 2-sphere  $S^2$ , one follows the same steps as in the previous section, with the difference that the  $L^2$  orthogonal basis on the sphere is provided by the spherical harmonics  $Y_{l,m}(\vartheta, \phi)$ , with  $\vartheta \in [0, \pi]$ ,  $\phi \in [0, 2\pi)$  and  $\ell = 0, 1, 2, \dots$ ,  $m = -l, \dots, l$ . We decompose the vorticity function in the spherical harmonics basis  $\omega(t, \vartheta, \phi) = \sum_{\ell, m} \omega^{\ell, m}(t) Y_{\ell, m}(\vartheta, \phi)$  and insert the decomposition into the Euler equations (4.5), which yields the following dynamical system for the modified coefficients  $\omega_{\ell, m} = i(-1)^m \omega^{\ell, -m}$  (the indices  $\ell, \ell', \ell''$  run all the way up to  $+\infty$ ):

$$\dot{\omega}_{\ell, m} = - \sum_{\ell', m'} \sum_{\ell'', m''} (-1)^{m'} \frac{\omega_{\ell', -m'} \omega_{\ell'', m''}}{\ell'(\ell' + 1)} \gamma_{\ell m, \ell' m'}^{\ell'' m''}, \quad (4.30)$$

where  $\gamma_{\ell m, \ell' m'}^{\ell'' m''}$  are the structure constants of the Lie algebra of divergence-free vector fields  $\mathcal{D}_\mu(S^2)$  on  $S^2$  realized as a Lie algebra of functions on  $S^2$  with the Lie algebra structure being the Poisson bracket:

$$i\{Y_{\ell, m}, Y_{\ell', m'}\} = \sum_{\ell'', m''} \gamma_{\ell m, \ell' m'}^{\ell'' m''} Y_{\ell'', m''}.$$

Similar to the case of the torus  $\mathbb{T}^2$ , there exists a representation of the algebra of skew-hermitian matrices  $\mathfrak{u}(N)$  (or  $\mathfrak{su}(N)$  if one removes  $\omega^{00}$  to keep the fields zero-mean) with structure constants approximating  $\gamma_{\ell', m'}^{\ell'' m''}$ , see for details [24, 25]. The matrices

$$(T_{\ell m}^N)_{m_1 m_2} = (-1)^{[(N-1)/2] - m_1} \sqrt{2\ell + 1} \begin{pmatrix} \frac{N-1}{2} & \ell & \frac{N-1}{2} \\ -m_1 & m & m_2 \end{pmatrix},$$

with  $(:::)$  standing for the Wigner 3j-symbol, are called *matrix harmonics*. They form a basis in  $\mathfrak{u}(N)$ , with the structure constants  $f_{\ell m, \ell' m'}^{(N)\ell'' m''}$ , arising from the commutation relations,

$$[T_{\ell m}^N, T_{\ell' m'}^N] = \sum_{\ell'' m''} f_{\ell m, \ell' m'}^{(N)\ell'' m''} T_{\ell'' m''}^N,$$

and given by the formula

$$\begin{aligned} f_{\ell m, \ell' m'}^{(N)\ell'' m''} &= (1 - (-1)^{\ell + \ell' + \ell''}) (-1)^{m'' + 1} \sqrt{(2\ell + 1)(2\ell' + 1)(2\ell'' + 1)} \\ &\times \begin{pmatrix} \ell & \ell' & \ell'' \\ m & m' & m'' \end{pmatrix} \left\{ \begin{matrix} \ell & \ell' & \ell'' \\ \frac{N-1}{2} & \frac{N-1}{2} & \frac{N-1}{2} \end{matrix} \right\}, \end{aligned}$$

where  $\{:::\}$  is the Wigner 6j-symbol.

Under a suitable normalization [24], the structure constants  $f_{\ell m, \ell' m'}^{(N)\ell'' m''}$  of  $\mathfrak{su}(N)$  tend to those of  $\mathcal{D}_\mu(S^2)$ .

Truncating the equations (4.30) at some level  $N$  and modifying the structure constants  $\gamma_{\ell m, \ell' m'}^{\ell'' m''} \mapsto f_{\ell m, \ell' m'}^{(N)\ell'' m''}$ , we get the system of the *Euler–Zeitlin equations* approximating the Euler equations on the sphere:

$$\dot{\omega}_{\ell, m} = - \sum_{\ell'=1}^{N-1} \sum_{\ell''=1}^{N-1} \sum_{m'=-\ell'}^{\ell'} \sum_{m''=-\ell''}^{\ell''} (\ell'(\ell' + 1))^{-1} f_{\ell m, \ell' m'}^{(N)\ell'' m''} (-1)^{m'} \omega_{\ell', -m'} \omega_{\ell'', m''}. \quad (4.31)$$

Similar to the case of the flat torus, we introduce the matrices

$$W = \sum_{\ell=1}^{N-1} \sum_{m=-\ell}^{\ell} i\omega^{\ell, m} T_{\ell m}^N, \quad P = \Delta_N^{-1}(W),$$

and rewrite the equations (4.31) in a compact matrix form:

$$\dot{W} = [W, P], \quad W = \Delta_N P, \quad W, P \in \mathfrak{su}(N). \quad (4.32)$$

The operator  $\Delta_N: \mathfrak{su}(N) \rightarrow \mathfrak{su}(N)$  is called the *Hoppe–Yau Laplacian*, see [25]. It is constructed from the double brackets of matrix harmonics  $T_{\ell m}^N$ , and its eigenvalues coincide with those of the Laplace operator  $\Delta$  on the sphere, i.e.  $\Delta_N T_{\ell m}^N = -\ell(\ell+1)T_{\ell m}^N$ . We thus obtain the same dynamical system for the Euler equations on the sphere, as for that on the flat torus. The difference lies in the bases of  $\mathfrak{su}(N)$  that are used to reconstruct the corresponding fields  $\omega(t, \mathbf{x})$  on  $\mathbb{T}^2$  and  $\omega(t, \vartheta, \phi)$  on  $S^2$ , and also in the discrete Laplacian  $\Delta_N$ . We conclude this section with the theorem summarizing the Hamiltonian nature of equations (4.32).

**Theorem 4.4.** *The Euler–Zeitlin equation (4.32) constitute a Lie–Poisson flow on the dual of the Lie algebra  $\mathfrak{su}(N)$ . The quantities*

$$C_m^N = \frac{4\pi}{N} \text{tr}(W^m), \quad m = 1, 2, \dots, N$$

are Casimirs for (4.32), and the quantity

$$H^N = \frac{2\pi}{N} \text{tr}(WP)$$

is the Hamiltonian.

The analogous truncation of MHD on the sphere, which we call *MHD–Zeitlin equations*, is discussed in detail in Paper I.

Since their derivation, the structure preserving finite-mode truncations have drawn a lot of attention. In particular, the problem of finding a suitable time integrator for the sine-Euler and the Euler–Zeitlin equations perfectly fits the realm of geometric numerical integration, and a fast integrator for them was developed by McLachlan [31] and later by Modin and Viviani [36]. The difference in the statistical behavior between simulations of turbulence by standard methods and sine-truncations was studied in [2, 16, 26]. Convergence of the sine truncations on the torus was proved in [14], and on the sphere in [37].



## 5 Summary of included papers

### 5.1 Paper I

In Paper I, we develop a spatio-temporal discretization for MHD on the sphere that fully preserves the underlying Lie–Poisson geometry. This includes extension of the Euler–Zeitlin model to MHD resulting in a finite-dimensional Lie–Poisson system, and further discretization in time leading to a Lie–Poisson integrator for semidirect product Lie algebras.

First, we use the vorticity formulation of MHD (2.46) on the sphere  $S^2$  in terms of four scalar fields, two vorticity fields  $\omega$  and  $\beta$  for the velocity and magnetic fields respectively, and two stream functions  $\psi$  and  $\theta$ :

**Proposition 5.1.** *The vorticity formulation for incompressible MHD equations (2.46) is*

$$\begin{cases} \dot{\omega} = \{\omega, \psi\} + \{\theta, \beta\}, & \omega = \Delta\psi, \\ \dot{\theta} = \{\theta, \psi\}, & \beta = \Delta\theta, \end{cases} \quad (5.1)$$

where  $\{\cdot, \cdot\}$  is a Poisson bracket on  $S^2$ .

Then, based on *Berezin–Toeplitz quantization*, we provide a spatially discrete analogue of (5.1), which is a Lie–Poisson system on the dual of the semidirect product Lie algebra  $\mathfrak{f}^* = \mathfrak{su}(N) \ltimes \mathfrak{su}(N)^*$ :

$$\begin{cases} \dot{W} = [W, M_1] + [\Theta, M_2], \\ \dot{\Theta} = [\Theta, M_1], \end{cases} \quad (5.2)$$

where  $W, \Theta \in \mathfrak{su}(N)$ ,  $M_1 = \Delta_N^{-1}W$ ,  $M_2 = \Delta_N\Theta$ , and  $\Delta_N: \mathfrak{su}(N) \rightarrow \mathfrak{su}(N)$  is the Hoppe–Yau Laplacian.

**Proposition 5.2.** *System (5.2) is a Lie–Poisson flow on the dual  $\mathfrak{f}^*$  of the Lie algebra  $\mathfrak{f} = \mathfrak{su}(N) \ltimes \mathfrak{su}(N)^*$ :*

$$\dot{J} = \text{ad}_M^* J,$$

where  $J = (\Theta, W^\dagger) \in \mathfrak{f}^*$ ,  $M = (M_1, M_2^\dagger) \in \mathfrak{f}$ , with the Hamiltonian

$$H(W, \Theta) = \frac{1}{2} (\text{tr}(W^\dagger M_1) + \text{tr}(\Theta^\dagger M_2)). \quad (5.3)$$

The functions

$$\mathcal{C}_f^N(\Theta) = \frac{4\pi}{N} \text{tr}(f(\Theta)), \quad \mathcal{I}_g^N(W, \Theta) = \frac{4\pi}{N} \text{tr}(Wg(\Theta)), \quad (5.4)$$

for arbitrary smooth functions  $f$  and  $g$ , are Casimirs for (5.2).

Further, we develop discrete Lie–Poisson reduction for semidirect products that can be summarized in the diagram Fig. 3.7.

**Proposition 5.3.** *The canonical equations on  $T^*F$*

$$\begin{cases} \dot{Q} = -M_1 Q, \\ \dot{P} = M_1^\dagger P + 2M_2^\dagger Q \alpha^\dagger, \\ \dot{\alpha} = 0, \end{cases} \quad (5.5)$$

with right-invariant Hamiltonian  $\tilde{H} = H \circ \mu$ , where

$$M_1 = \Delta_N^{-1} W, \quad M_2 = \Delta_N \Theta, \quad H(W, \Theta) = \frac{1}{2} (\text{tr}(W^\dagger M_1) + \text{tr}(\Theta^\dagger M_2)),$$

are reduced to the Lie–Poisson system on  $\mathfrak{f}^*$

$$\dot{W} = [W, M_1] + [\Theta, M_2], \quad \dot{\Theta} = [\Theta, M_1], \quad (5.6)$$

by means of the momentum map (2.23).

We use the implicit midpoint method (3.5) as a symplectic scheme on  $T^*F$  and prove that it descends to a Lie–Poisson integrator on  $\mathfrak{f}^*$ , and arrive at the main result.

**Theorem 5.1.** *The implicit midpoint method (3.5) for the Hamiltonian system (5.5) descends to a Lie–Poisson integrator  $\phi_h: \mathfrak{f}^* \rightarrow \mathfrak{f}^*$ ,  $\phi_h: (W_n, \Theta_n) \mapsto (W_{n+1}, \Theta_{n+1})$  for the Lie–Poisson flow (5.2). The method is given explicitly by the following formulas:*

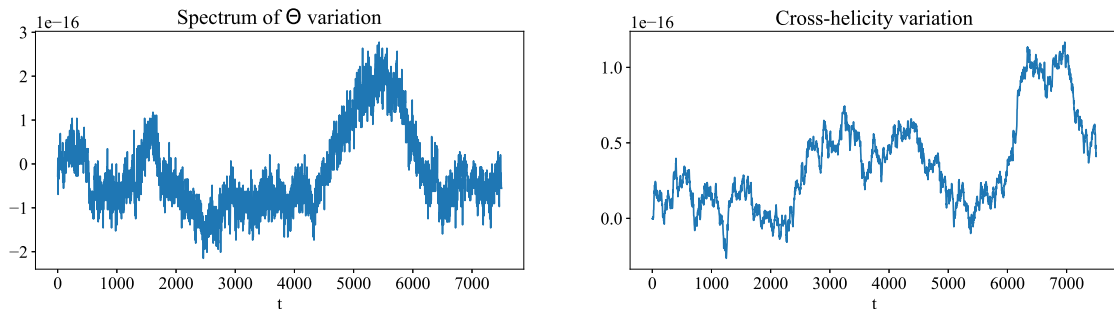
$$\begin{aligned} \Theta_n &= \tilde{\Theta} - \frac{h}{2} [\tilde{\Theta}, \tilde{M}_1] - \frac{h^2}{4} \tilde{M}_1 \tilde{\Theta} \tilde{M}_1, \\ \Theta_{n+1} &= \Theta_n + h [\tilde{\Theta}, \tilde{M}_1], \\ W_n &= \tilde{W} - \frac{h}{2} [\tilde{W}, \tilde{M}_1] - \frac{h}{2} [\tilde{\Theta}, \tilde{M}_2] - \frac{h^2}{4} (\tilde{M}_1 \tilde{W} \tilde{M}_1 + \tilde{M}_2 \tilde{\Theta} \tilde{M}_1 + \tilde{M}_1 \tilde{\Theta} \tilde{M}_2), \\ W_{n+1} &= W_n + h [\tilde{W}, \tilde{M}_1] + h [\tilde{\Theta}, \tilde{M}_2], \end{aligned} \quad (5.7)$$

where  $\tilde{M}_1 = \Delta_N^{-1}(\tilde{W})$ ,  $\tilde{M}_2 = \Delta_N(\tilde{\Theta})$ .

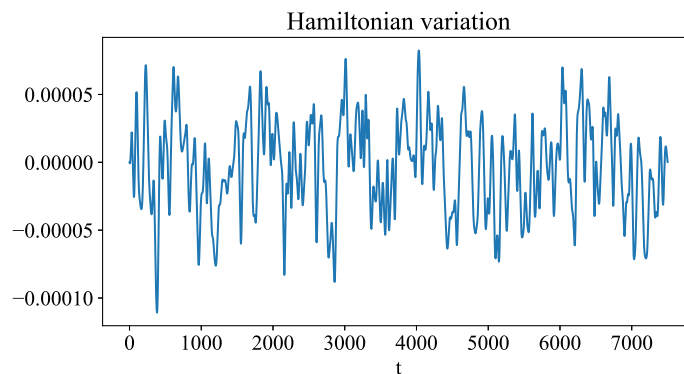
The integrator (5.7) preserves the Casimirs (5.4):

$$\begin{aligned} \text{tr}(f(\Theta_n)) &= \text{tr}(f(\Theta_{n+1})), \\ \text{tr}(W_n g(\Theta_n)) &= \text{tr}(W_{n+1} g(\Theta_{n+1})). \end{aligned}$$

Numerical simulations confirm that the method has all the properties indicated in Theorem 5.1. Variations of the Casimir functions shown in Fig. 5.1 indicate their exact preservation, as the magnitude  $10^{-16}$  is the tolerance of the fixed point iterations. Also, we observe near preservation of the Hamiltonian function in Fig. 5.2.



**Fig. 5.1.** Variation of the smallest eigenvalue of  $\Theta$  (left), and cross-helicity  $\text{tr}(W\Theta)$  (right) for incompressible MHD equations. The order  $10^{-16}$  of the magnitude of the variation indicates the exact preservation of the Casimirs.



**Fig. 5.2.** Variation of the Hamiltonian for incompressible MHD equations. Absence of drift indicates nearly preservation of the Hamiltonian.

## 5.2 Paper II

In Paper II, we apply the structure preserving discretization for MHD developed in Paper I to study the dynamics of magnetized fluids given by Hazeltine's model [21, 17, 18, 19], as well as its two limiting models, reduced MHD (RMHD) and the Charney–Hasegawa–Mima (CHM) model. Hazeltine's equations generalize the MHD system (5.1):

$$\begin{cases} \dot{\omega} = \{\omega, \psi\} + \{\theta, j\}, & \omega = \Delta\psi, \\ \dot{\theta} = \{\theta, \psi\} - \alpha\{\theta, \chi\}, & j = \Delta\theta. \\ \dot{\chi} = \{\chi, \psi\} + \{\theta, j\}, \end{cases} \quad (5.8)$$

where  $\omega$  and  $\theta$  have the same meaning as before,  $\chi$  is the normalized deviation of particle density from a constant equilibrium value, and  $\alpha$  is a constant parameter.

The Zeitlin equations for (5.8) are

$$\begin{cases} \dot{Q} = \frac{1}{\hbar}[Q, P], \\ \dot{\Theta} = \frac{1}{\hbar}[\Theta, P - \alpha R], \\ \dot{R} = \frac{1}{\hbar}[R, P] + \frac{1}{\hbar}[\Theta, J], \end{cases} \quad (5.9)$$

where  $R \in \mathfrak{su}(N)$  is the matrix for the field  $\chi$ ,  $P \in \mathfrak{su}(N)$  is the matrix for the field  $\psi$ ,  $J \in \mathfrak{su}(N)$  is the matrix for the field  $j$ ,  $Q = W - R$ ,  $\hbar = 2/\sqrt{N^2 - 1}$ .

**Proposition 5.4.** *System (5.9) is a Lie–Poisson flow on the dual  $\mathfrak{f}^*$  of the Lie algebra*

$$\mathfrak{f} = \mathfrak{su}(N) \oplus (\mathfrak{su}(N) \ltimes \mathfrak{su}(N)^*)$$

with the Casimir invariants

$$\mathcal{C}_f^N = \frac{4\pi}{N} \text{tr}(f(\Theta)), \quad \mathcal{I}_g^N = \frac{4\pi}{N} \text{tr}(Rg(\Theta)), \quad \mathcal{P}_h^N = \frac{4\pi}{N} \text{tr}(k(Q)), \quad (5.10)$$

for arbitrary smooth functions  $f, g, k$ , and the Hamiltonian

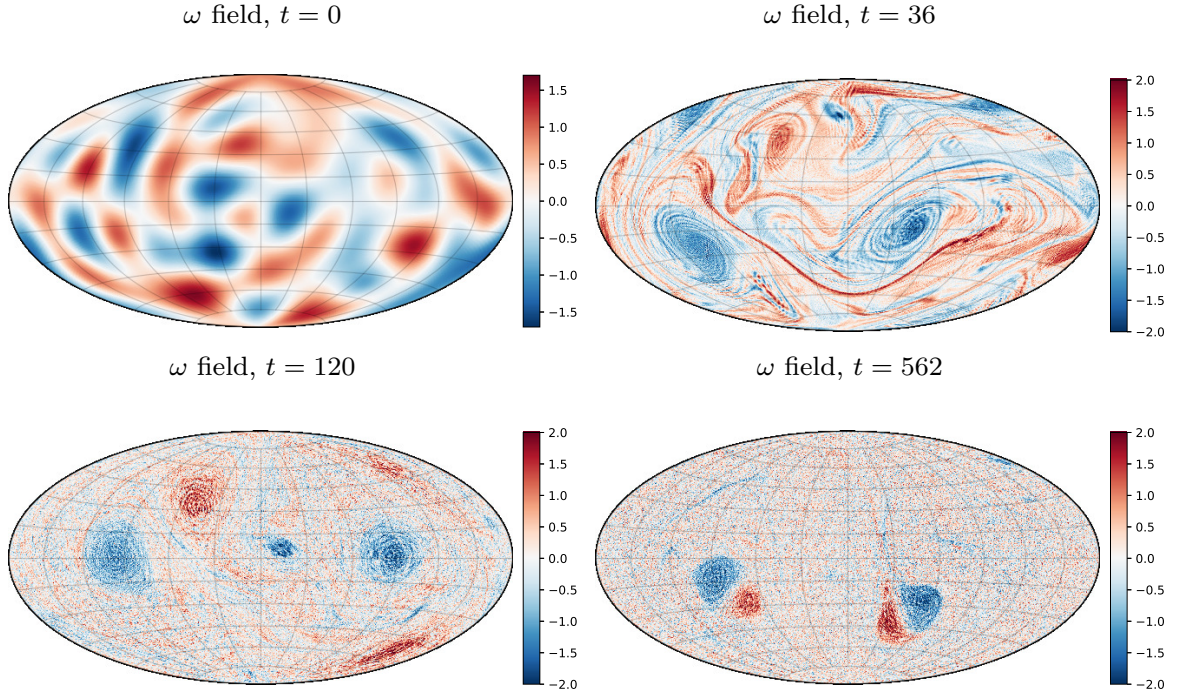
$$H = \frac{2\pi}{N} \text{tr}(W^\dagger P + \Theta^\dagger J - \alpha R^\dagger R). \quad (5.11)$$

A structure preserving integrator for (5.9) is given by

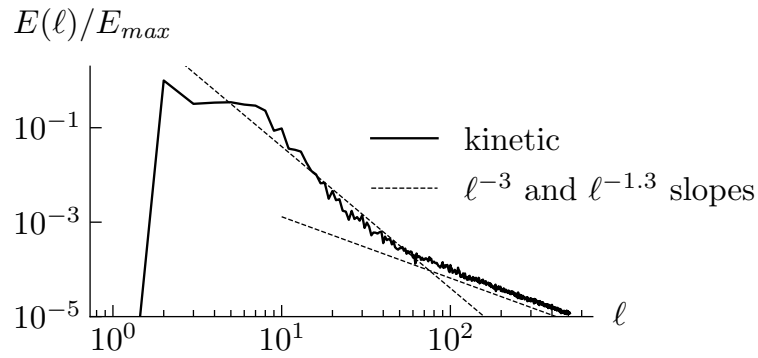
$$\begin{aligned} \Theta_n &= \tilde{\Theta} - \frac{\varepsilon}{2}[\tilde{\Theta}, \tilde{M}] - \frac{\varepsilon^2}{4}\tilde{M}\tilde{\Theta}\tilde{M}, \\ \Theta_{n+1} &= \Theta_n + \varepsilon[\tilde{\Theta}, \tilde{M}], \\ Q_n &= \tilde{Q} - \frac{\varepsilon}{2}[\tilde{Q}, \tilde{P}] - \frac{\varepsilon^2}{4}\tilde{P}\tilde{Q}\tilde{P}, \\ Q_{n+1} &= Q_n + \varepsilon[\tilde{Q}, \tilde{P}], \\ R_n &= \tilde{R} - \frac{\varepsilon}{2}[\tilde{R}, \tilde{M}] - \frac{\varepsilon}{2}[\tilde{\Theta}, \tilde{J}] - \frac{\varepsilon^2}{4}(\tilde{M}\tilde{R}\tilde{M} + \tilde{J}\tilde{\Theta}\tilde{M} + \tilde{M}\tilde{\Theta}\tilde{J}), \\ R_{n+1} &= R_n + \varepsilon[\tilde{R}, \tilde{M}] + \varepsilon[\tilde{\Theta}, \tilde{J}], \end{aligned} \quad (5.12)$$

where  $\tilde{M} = \tilde{P} - \alpha\tilde{R}$  and  $\varepsilon = \delta t/\hbar$  is the physical time step length  $\delta t > 0$ . Similar to the integrator (5.7), the scheme (5.12) preserves the Casimirs (5.10) and nearly preserves the Hamiltonian (5.11).

Typical snapshots of simulations for Hazeltine’s equations are shown in Fig. 5.3. They indicate presence of the inverse kinetic energy cascade, which is shown in energy spectral diagrams, see Fig. 5.4.



**Fig. 5.3. Hazeltine:** Evolution of the vorticity  $\omega(t)$  field. Smooth randomly generated initial vorticity distribution evolves into vortex blob configuration on the small scale background noise.



**Fig. 5.4. Hazeltine:** Kinetic energy spectrum of the final state at  $T = 562$ . The spectrum has a broken line shape with the scaling  $l^{-3}$  for the low frequency part, and  $l^{-1.3}$  for the high frequency part.

### 5.3 Paper III

In Paper III, we derive the global model of thermal quasi-geostrophy (TQG) on the sphere from the thermal rotating shallow water (TRSW) equations. The obtained

TQG model reads:

$$\begin{cases} \dot{q} = \{q, \psi\} + \{b, j\}, \\ \dot{b} = \{b, \psi\}, \\ q = (\Delta - \gamma\mu^2)\psi + \frac{2\mu}{\text{Ro}} - \mu h_1 + \mu b, \\ j = h_1 - \mu\psi. \end{cases} \quad (5.13)$$

where  $q$  is the potential vorticity,  $b$  is the buoyancy,  $\gamma$  is the Lamb parameter, and  $\text{Ro}$  is the Rossby number.

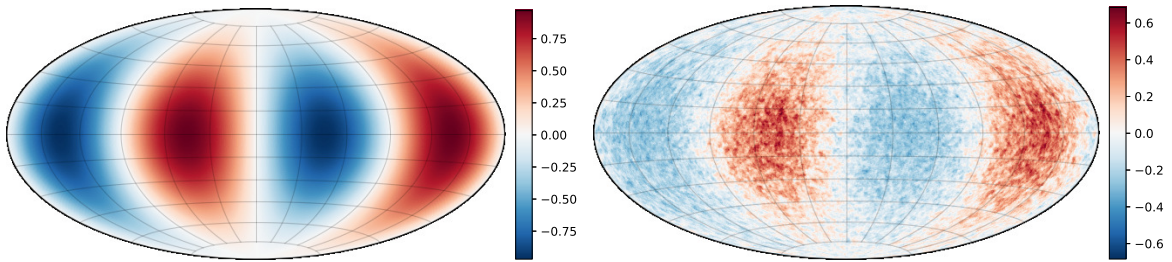
Conserved quantities for (5.13) are Hamiltonian

$$\begin{aligned} H = & \frac{1}{2} \int_{S^2} \left( q - \frac{2\mu}{\text{Ro}} + \mu(h_1 - b) \right) \cdot (\Delta - \gamma\mu^2)^{-1} \left( q - \frac{2\mu}{\text{Ro}} + \mu(h_1 - b) \right) dx dy + \\ & + \int_{S^2} b h_1 dx dy = \frac{1}{2} \int_{S^2} \left( q - \frac{2\mu}{\text{Ro}} + \mu(h_1 - b) \right) \psi dx dy + \int_{S^2} b h_1 dx dy, \end{aligned} \quad (5.14)$$

as well as Casimir invariants

$$\mathcal{C}_f = \int_{S^2} f(b) dx dy, \quad \mathcal{I}_g = \int_{S^2} qg(b) dx dy, \quad (5.15)$$

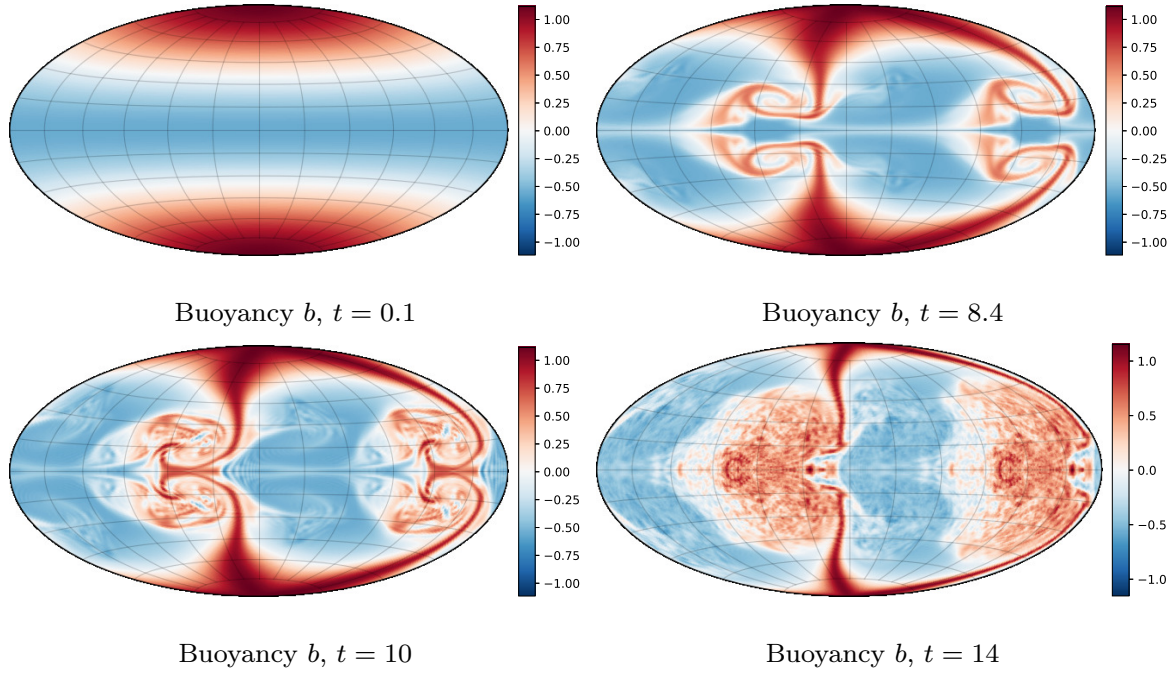
where  $f$  and  $g$  are arbitrary smooth functions. One observes similarities between the TQG (5.13) and RMHD (5.1) models. Indeed, they share the Hamiltonian formulation in terms of the semidirect product Lie–Poisson bracket. This allows to utilize the methods developed in Paper I to study the global TQG dynamics. Large-scale flow patterns revealed intricate dynamic interplay between potential vorticity, buoyancy, and bathymetry, which is shown in Fig. 5.6 and Fig. 5.5.



**Fig. 5.5.** Adopted bathymetry profile (left) and final distribution of the buoyancy (right). The buoyancy aligns with the bathymetry.

## 5.4 Paper IV

In paper IV, we extend the matrix approach to MHD from two dimensions to axially symmetric flows on the three-sphere  $S^3$ . The key idea is to make use of



**Fig. 5.6.** Buoyancy dynamics. From an initially smooth field, mushroom-like dipole structures form and roll up asymmetrically under the influence of rotation and the interaction with the bathymetry. Circulation is induced via the buoyancy-bathymetry interaction and turbulence is generated which eventually aligns with the bathymetry.

the Hopf fibration and is summarized as follows: the quotient of the action of the Hopf field on  $S^3$  is the two-dimensional sphere  $S^2$ , and therefore if one assumes the  $S^1$ -symmetry, generated by the Hopf field, of solutions to MHD on  $S^3$ , one gets the symmetry reduced version of three-dimensional MHD on the two-sphere.

The system of self-consistent MHD describes the evolution of a divergence-free velocity field  $u(t, x)$  and magnetic field  $B(t, x)$  on a three-dimensional Riemannian manifold  $(M, g) \ni x$ :

$$\begin{cases} \dot{u} + \nabla_u u = -\nabla p + \text{curl} B \times B, \\ \dot{B} = \text{curl}(u \times B), \\ \text{div} B = 0, \\ \text{div} u = 0, \end{cases} \quad (5.16)$$

where  $p(t, x)$  is the pressure function,  $\nabla_u u$  is the covariant derivative of the vector field  $u$  along itself. The term  $\text{curl} B \times B$  represents the Lorentz force, and the second equation in (5.16) reflects the frozenness of the magnetic field into the fluid.

The  $S^1$ -symmetry reduced version of equations (5.16) is

$$\begin{cases} \Delta\dot{\psi} = \{\Delta\psi, \psi\} + \{\xi, \Delta\xi\} + 2\{q, \psi\} + 2\{\xi, \rho\}, \\ \dot{\rho} = \{\rho, \psi\} + \{\xi, q\} + 2\{\psi, \xi\}, \\ \dot{q} = \{q, \psi\} + \{\xi, \rho\}, \\ \dot{\xi} = \{\xi, \psi\}, \end{cases} \quad (5.17)$$

where  $q, \psi, \rho, \xi \in C^\infty(S^2)$ , and  $\{\cdot, \cdot\}$  is the Poisson bracket on  $S^2$ .

The system (5.17) admits a Hamiltonian formulation outlined in the following theorem.

**Theorem 5.2.** *The system of axisymmetric MHD equations on  $S^3$  defined in (5.17) is a Lie–Poisson system on the dual  $\mathcal{F}^*$  of the Lie algebra*

$$\mathcal{F} = (\mathfrak{X}_\mu(S^2) \times C^\infty(S^2)) \times (\mathfrak{X}_\mu(S^2) \times C^\infty(S^2))^*,$$

with the Hamiltonian given by

$$H = -\frac{1}{2} \int_{S^2} (\psi \Delta\psi - q^2) \mu - \frac{1}{2} \int_{S^2} (\xi \Delta\xi - \rho^2) \mu. \quad (5.18)$$

**Proposition 5.5.** *The quantities*

$$\mathcal{I} = \int_{S^2} (\xi \Delta\psi - \rho q) \mu, \quad \mathcal{C}_f = \int_{S^2} f(\xi) \mu, \quad J_h = \int_{S^2} \rho h(\xi) \mu, \quad K_g = \int_{S^2} qg(\xi) \mu$$

are Casimir invariants for the system of axisymmetric MHD equations on  $S^3$  defined in (5.17). The energy (5.18) is also conserved by the flow (5.17).

Further, a matrix version of equations (5.17) is developed:

$$\begin{cases} \Delta\dot{\Psi} = \frac{1}{\hbar} [\Delta_N \Psi, \Psi] + \frac{1}{\hbar} [\Xi, \Delta_N \Xi] + \frac{2}{\hbar} [Q, \Psi] + \frac{2}{\hbar} [\Xi, P], \\ \dot{P} = \frac{1}{\hbar} [P, \Psi] + \frac{1}{\hbar} [\Xi, Q] + \frac{2}{\hbar} [\Psi, \Xi], \\ \dot{Q} = \frac{1}{\hbar} [Q, \Psi] + \frac{1}{\hbar} [\Xi, P], \\ \dot{\Xi} = \frac{1}{\hbar} [\Xi, \Psi], \end{cases} \quad (5.19)$$

where  $\Psi, Q, P, \Xi \in \mathfrak{su}(N)$ , and  $\Delta_N: \mathfrak{su}(N) \rightarrow \mathfrak{su}(N)$  is the Hoppe–Yau Laplacian.

The Hamiltonian formulation for (5.19) is given as well:

**Theorem 5.3.** *The axisymmetric MHD–Zeitlin equations (5.19) are Lie–Poisson on the dual  $\mathcal{F}^*$  of the Lie algebra  $\mathcal{F} = (\mathfrak{su}(N) \times \mathfrak{su}(N)) \times (\mathfrak{su}(N) \times \mathfrak{su}(N))^*$ , with the Hamiltonian function given by*

$$H^N = -\frac{2\pi}{N} \operatorname{tr}(\Psi(\Delta_N \Psi) - Q^2) - \frac{2\pi}{N} \operatorname{tr}(\Xi(\Delta_N \Xi) - P^2). \quad (5.20)$$

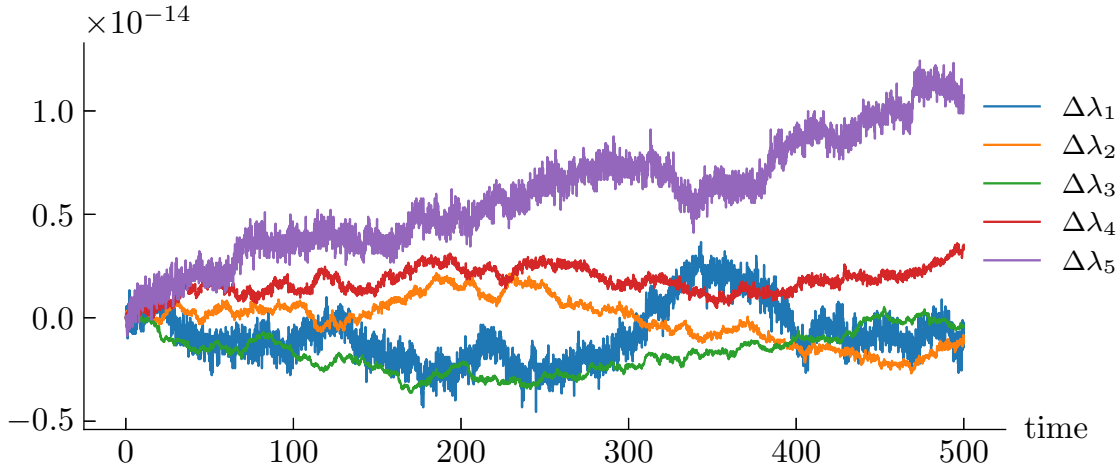
**Proposition 5.6.** *The following quantities are Casimir invariants for (5.19):*

$$\begin{aligned} \mathcal{I}^N &= \frac{4\pi}{N} \operatorname{tr}(\Xi(\Delta_N \Psi) - PQ), & \mathcal{C}_f^N &= \frac{4\pi}{N} \operatorname{tr}(f(\Xi)), \\ J_h^N &= \frac{4\pi}{N} \operatorname{tr}(Ph(\Xi)), & K_g^N &= \frac{4\pi}{N} \operatorname{tr}(Qg(\Xi)), \end{aligned}$$

for arbitrary functions  $f, g, h$ .

The Hamiltonian (5.20) is also conserved by the flow.

Further, a structure preserving time integrator for (5.19) is developed, and its preservation properties are shown in numerical simulations, for example, in Fig. 5.7.



**Fig. 5.7.** Preservation of the eigenvalues  $\lambda_1, \dots, \lambda_5$  of the matrix  $\Xi \in \mathfrak{su}(N)$  with  $N = 5$ . The magnitude  $10^{-14}$  of the variation  $\Delta\lambda_i = \lambda_i(t) - \lambda_i(0)$  of the eigenvalues shows that the spectrum of  $\Xi$  is preserved up to machine precision.



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