

GAUGE STRUCTURE IN  
ALGORITHMS FOR PLASMA PHYSICS

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# Abstract

In recent years, structure-preserving algorithms have proliferated in computational plasma physics. Such algorithms rigorously preserve geometric and topological features of the plasmas they model. This dissertation studies a particular feature of these algorithms, namely, their preservation of gauge symmetry and conservation laws—collectively described as their gauge structure. In this work, new extensions of Noether’s theorems are discovered in discrete settings, and a comprehensive theoretical grounding for charge conservation is thereby established for gauge-symmetric particle-in-cell (PIC) algorithms for plasma physics.

First, a new, general class of algorithms—gauge-compatible splitting methods—is discovered that exactly upholds the Noether principle in discrete Hamiltonian systems. Second, a method of this class is constructed for a PIC algorithm, whose electromagnetic gauge structure is systematically analyzed via the momentum map. Third, this result is extended to a PIC method defined using finite element exterior calculus, and it is tested numerically therewith. Fourth, a formulation of Noether’s second theorem is developed and applied toward a variational PIC algorithm using the formalism of discrete exterior calculus.

The successful preservation of electromagnetic gauge structure in discrete algorithms motivates the exploration of a related problem in the appendices of this thesis. In particular, while internal gauge symmetries are demonstrated to be well preserved in structure-preserving simulations of physical systems, their spacetime symmetries are crucially forfeited in algorithms that discretize the spacetime manifold. In plasma physics algorithms, the breaking of spacetime symmetry generally leads to an unfortunate loss of energy-momentum conservation.

While continuous spacetime and its symmetries are incompatible with discretely defined simulations, an alternative realization of these symmetries is more amenable to algorithmic description. In the appendices, a discrete field theory is pursued that

reinterprets the Poincaré symmetries of spacetime as internal gauge transformations. New finite-dimensional Poincaré representations are explored as the targets of such gauge transformations, and a method is developed to construct their matter currents. Further applying such a representation, a structure-preserving algorithm for gravitational simulations in vacuum is also derived from a novel discretization of the tetradic Palatini action.

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# 1

## Introduction

### 1.1 Motivations

Kinetic and fluid plasma models exhibit nonlinear interactions between charged particles and electromagnetic fields that are often intractable to analysis. In general, such models admit closed-form solutions only for plasma systems that have been judiciously simplified. As computational power advances, however, the properties and dynamics of more general systems of plasmas have become amenable to investigation. Computer simulations therefore play an increasingly important role in the study of plasma behavior.

Owing in part to the rich mathematical structure of plasma models, as well as the need for accuracy in simulations, *structure-preserving algorithms* [1, 2] have flourished in computational plasma physics in recent years. Such methods produce simulations that retain the geometric and topological structures of physical systems, including their symplectic structure, symmetries, conservation laws, and cohomology. Preserving these structures can improve the long-term accuracy of numerical simulations and more faithfully model the underlying physics of plasmas.

In the past decade, numerous structure-preserving algorithms for plasma simu-

lations have appeared in the literature, [e.g. 3–28]. Such methods model kinetic or hybrid fluid-kinetic plasmas employing either Lagrangian or Hamiltonian formalisms. In these sources, kinetic physics is simulated via the particle-in-cell (PIC) method, which has long been a workhorse for the study of fusion plasmas [29–31]. These studies further employ discretizations derived from discrete exterior calculus (DEC) [32, 33], finite element exterior calculus (FEEC) [34, 35], or close relatives (using Whitney forms [36, 37], for example) thereof.

A critical property of such algorithms, which will be systematically studied in this thesis, is their preservation of gauge symmetries and associated conservation laws—collectively described as their gauge structure. The symmetries that characterize a physical system are crucial in determining its dynamics and behavior. Algorithms that preserve gauge structure are correspondingly quite demanding; they are generally derived from a symplectic structure or variational principle, and they must employ spatial and time discretizations that preserve gauge symmetry. It turns out that such discretizations often necessitate the cohomological structure inherent in formalisms such as DEC and FEEC. In a sense, therefore, gauge structure is ‘deeply buried’ in the construction of physical systems; its preservation necessitates the preservation of many other structures of interest.

Gauge structure was first formalized in Noether’s theorems, published in 1918 [38]. Noether’s first theorem (N1T) famously established a correspondence between the symmetries of Lagrangian systems and their conservation laws, and Noether’s second theorem (N2T) established a correspondence between local gauge symmetries of degenerate Lagrangians and differential identities satisfied by their equations of motion. In their original setting, Noether’s theorems are constructed for Lagrangian systems in continuous spacetime. As a result, they are not immediately applicable to numerical algorithms, which necessarily describe physical systems as discrete, finite data sets.

To sharpen the nontriviality of applying Noether’s theorems to discrete systems, it is worth noting that Noether’s theorems are specifically addressed to smooth symmetries that infinitesimally transform a physical system. As an example, a circle is invariant under infinitesimal rotations by an arbitrarily small angle. Such a smooth symmetry is to be contrasted with a discrete symmetry, such as the invariance of a square under rotations by multiples of the finite angle  $90^\circ$ , about which Noether’s original theorems have nothing to say.

Despite the tension one might first suspect between the smoothness of Noether symmetries and the discreteness of simulation algorithms, they are, in fact, reconcilable. Indeed, in recent years N1T and N2T have both been rigorously demonstrated for gauge-symmetric, discrete Lagrangian systems in the finite difference formalism [39, 40]. This remarkable extensibility of Noether’s theorems to discrete settings motivates the construction of algorithms that rigorously preserve the gauge structure of physical systems.

Noether’s theorems’ extensibility to the discrete domain appears somewhat more natural, perhaps, when a distinction is drawn between symmetries that transform physical quantities “vertically” (or “internally”), and those that transform “horizontally” (see Fig. 1.1). This dissertation shall use the term *gauge symmetry* to refer exclusively to vertical symmetries, which transform physical objects at fixed points in spacetime.<sup>(\*)</sup> Horizontal symmetries, on the other hand, are those which transform different points of spacetime into one another. This latter category includes the symmetries of spacetime itself—namely, the translations, rotations and boosts that comprise the Poincaré group. It is precisely gauge symmetries—and not spacetime symmetries—whose compatibility with Noether’s theorems has been demonstrated in

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<sup>(\*)</sup> The term “gauge symmetry” has varying uses in the literature. Amidst an effort to unify electricity and gravitation, Hermann Weyl first established the term in 1929 [41] to refer to “local” symmetries—those that depend on an arbitrary function of spacetime. In the context of general relativity, for example, spacetime symmetries are gauge symmetries in Weyl’s sense. The usage adopted here is restricted, however, to local *vertical* symmetries, a definition that hews more closely to the mathematical literature characterizing principal bundles [42, 43].

a discrete setting.

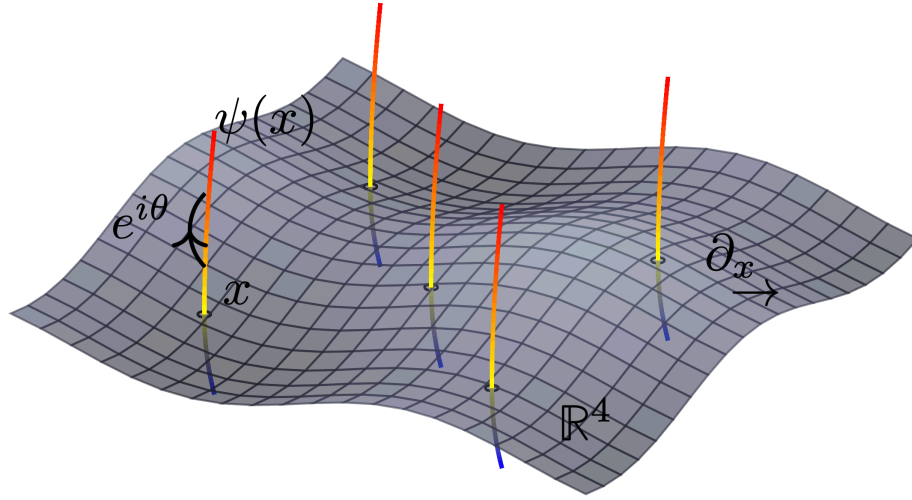


Figure 1.1: Vertical gauge symmetries are to be contrasted with horizontal spacetime symmetries. Spacetime is portrayed above as a surface to which “fibers” have been attached at each point. (Only an illustrative handful of fibers are shown.) An internal gauge symmetry is depicted as a map *within* the fiber attached to a fixed point  $x$ , which multiplies a field  $\psi(x)$  by a complex phase. A horizontal spacetime symmetry, by contrast, is a map between different points of the spacetime manifold.

As an example that is central to this dissertation, the gauge symmetry of electromagnetism is amenable to Noether’s theorem in both continuous and algorithmic settings. Indeed, in recent years, several PIC algorithms have been explored in the plasma physics literature whose simulations of particles and electromagnetic fields exactly conserve charge [3–6, 8, 9, 12–28]. Many of these references rightly observe that their method’s gauge symmetry guarantees its exact charge conservation, but this fact is often unproven; the associated conservation laws are not always stated, let alone systematically derived. The absence of such derivations motivates a rigorous study of algorithmic conservation laws in structure-preserving PIC methods.

Moreover, while Noether’s theorems have been formally demonstrated for discrete *variational* systems [39, 40], their rigorous demonstration for general discrete *Hamiltonian* systems has not yet appeared in the literature. This dissertation addresses this gap by identifying a new class of Hamiltonian splitting algorithms that exactly up-

hold the Noether principle—and its attendant conservation laws. Such a classification better explains why the literature’s aforementioned Hamiltonian PIC algorithms conserve charge, and offers a means to generalize their construction to other Hamiltonian systems.

From a more philosophical perspective, the study of gauge structure in algorithms, and of their mathematical structure in general, may be viewed as a small part of a larger effort to reconcile physical theory with modern tools of research. When Newton and Leibniz invented calculus in the late 1600s, it was a language well-suited to the tools of scholarship at hand—namely, pen and paper. Over three centuries later, as computers become ever more essential to progress in physics research, there is a stark mismatch between the continuous, infinitesimal language that Newton established for physics, and the discrete, digital language of physicists’ most powerful research tool. As the era of exascale computing approaches, the potential benefits of reconciling this mismatch continue to grow.

The field of computational physics has adapted to this apparent difficulty in creative and remarkable ways. This thesis will describe some of these bridges between computation and physical law as well as construct a few more. Nevertheless, the field faces a critical challenge: From plasma physics, to general relativity, to quantum field theory, the models of contemporary physics are defined against a background of continuous spacetime. The necessarily discrete spacetimes of computer algorithms not only lose information in their approximation of this continuum, they break the spacetime symmetries that give rise to the conservation of energy and momentum. These conservation laws are so foundational to physics that their absence—from even the most advanced algorithms—imposes a severe limitation on the ability of computational physics to genuinely reflect fundamental physical laws.

At the same time, the longstanding irreconcilability of general relativity and quantum field theory leaves considerable theoretical questions as to the nature of spacetime

at its smallest scales.

These twin computational and theoretical challenges invite attempts toward an intrinsically discrete characterization of fundamental physics. Such explorations might at least yield productive algorithms for the approximate simulation of existing physical laws. At best, they may lead to reformulations of physical laws in a language accessible to the computer.

## 1.2 Main contributions

The main contributions of this dissertation can be enumerated as follows:

1. By discovering a general class of splitting algorithms—gauge-compatible splitting methods—the Noether principle is rigorously demonstrated to hold in discrete Hamiltonian systems via preservation of the momentum map.
2. This classification is applied in the construction of a new gauge-compatible Hamiltonian PIC algorithm with a canonical Poisson bracket. This algorithm is further extended to the formalism of finite element exterior calculus—rendering it suitable for simulation on an unstructured mesh—and it is tested numerically.
3. The efficacy of Noether’s second theorem is demonstrated in the formalism of discrete exterior calculus, leading to the derivation of an off-shell charge continuity equation for a variational PIC method.

The appendix of this thesis makes a further contribution:

4. In pursuit of a discrete field theory that locally conserves energy-momentum, spacetime’s Poincaré symmetries are reinterpreted as internal gauge symmetries of physical fields. A new construction of matter currents using finite-dimensional Poincaré representations is discovered. A structure-preserving algorithm for vacuum gravitational simulations is also derived from a novel discretization of the tetradic Palatini action.

In greater detail, this dissertation systematically studies gauge-structure-preserving algorithms for plasma physics. It focuses largely on the construction of PIC algorithms that preserve the electromagnetic gauge symmetry of plasmas, thereby ensuring their conservation of electric charge.

Gauge structure preservation is first explored in Hamiltonian algorithms. The Hamiltonian counterpart of Noether’s theorems is encapsulated in a Hamiltonian system’s *momentum map* (sometimes named *moment map*),  $\mu$  [44–46]. The time-invariance of the momentum map— $\dot{\mu} = 0$ —is the Hamiltonian equivalent of a local Noether conservation law. In this dissertation, a novel, general class of algorithms is defined—*gauge-compatible splitting methods* [19]—whose preservation of the momentum map in gauge-symmetric Hamiltonian systems is rigorously demonstrated. This classification provides a Hamiltonian counterpart to the rigorous Noether’s theorem derived in discrete Lagrangian systems [39, 40].

The simple but effective characterization of gauge-compatible splitting methods is given as follows:

**Theorem [19]** Let  $\Phi$  be a canonical group action of a Lie group  $G$  on Poisson manifold  $M$  with momentum map  $\mu$ , and let  $H : M \rightarrow \mathbb{R}$  satisfy  $\Phi_g^* H = H, \forall g \in G$ . Suppose a splitting method  $H = \sum_{i=1}^N H_i$  satisfies:

- (1)  $\Phi_g^* H_i = H_i, \forall i$  and  $g \in G$ ;
- (2) subsystem  $H_i$  is solved exactly  $\forall i$ .

Then  $\mu$  is exactly preserved by the splitting method—that is,  $\dot{\mu} = 0$ .

This general classification is applied to the construction of a new Hamiltonian PIC method with a canonical Poisson bracket. Its charge conservation law is rigorously derived via the momentum map. In addition to its identification of the conserved charge and current associated with gauge symmetry, the importance of the momentum map is further demonstrated by its helpful determination of the appropriate initial conditions [19]. Lastly, the relationship between this PIC algorithm and existing methods in the literature (especially Xiao *et al.* [8]) is further clarified by studying its symplectic reduction.

The development of gauge-compatible splitting PIC methods is then extended to the FEEC formalism, resulting in a canonical bracket PIC algorithm suitable for simulation on an unstructured mesh. Initial conditions are optimized using insights gleaned from the algorithm’s momentum map, and two numerical tests of this algorithm are successfully simulated—a Landau damping simulation (see Fig. 1.2) as well as a simulation of the Weibel instability. [28].

The charge conservation law of a Lagrangian PIC method constructed in the DEC formalism [3] is then studied. The finite-difference N2T formalism of [40] is extended to a DEC setting. In this way, a discrete charge conservation law [19] for this method

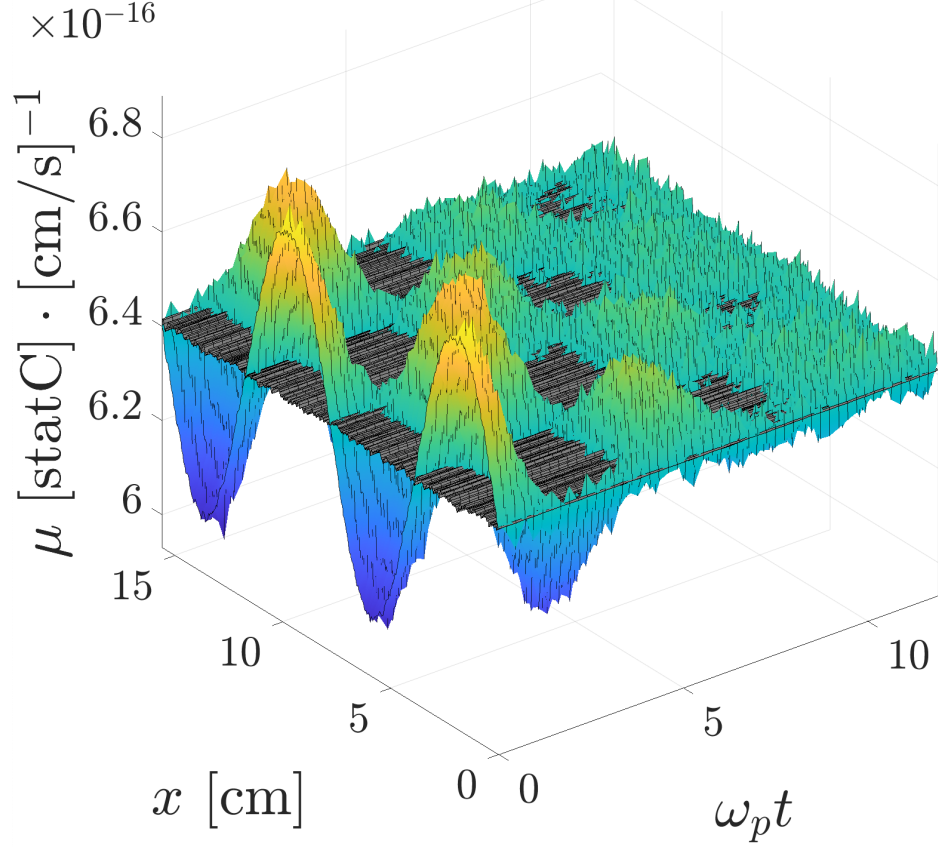


Figure 1.2: While the multicolor surface depicts the Landau damping of electron charge density over the lifetime of a simulation, the momentum map, depicted in gray, is exactly conserved at each point of the simulation domain.

is rigorously derived:

$$0 = \left( \rho_{n+\frac{1}{2}}^i - \rho_{n-\frac{1}{2}}^i \right) + \sum_j J^{[ij]}. \quad (1.1)$$

While the aforementioned efforts describe electromagnetic gauge symmetry, this symmetry comprises only one dimension of the larger symmetry group of plasma systems. In particular, plasmas are described in continuous spacetime, and therefore have spacetime symmetry. The ten Poincaré symmetries— $SO(3, 1) \times \mathbb{R}^4$ , defined by three rotations, three Lorentz boosts, and four spacetime translations—give rise to plasmas' conservation of angular momentum, the uniform trajectory of their relativis-

tic centers of mass, and to their conservation of linear energy-momentum, respectively. The preservation of these symmetries in algorithms for plasma physics would enable simulations that exactly conserve charge as well as these ten energy-momentum invariants.

The appendices to this dissertation describe the results of an effort to incorporate this symmetry in discrete algorithms [47–50]. The approach taken emphasizes a reinterpretation of the spacetime symmetries as internal gauge symmetries; certain theoretical strides are made that may prove useful to future studies of symmetry-preserving discrete field theories. One additional consequence of this effort is a novel structure-preserving algorithm for the simulation of gravitational systems in vacuum, derived from a Poincaré lattice gauge-theoretic discretization of the tetradic Palatini action.

Any Poincaré representation that is suitable for computation must be finite dimensional. Such a Poincaré representation is discovered as a contribution of this dissertation—namely, a 5-dimensional real representation called the *5-vector*, denoted  $\Phi$ . This matter field gauge-transforms under the left group action of a Poincaré group element  $g = (\Lambda, \varphi) \in SO(3, 1) \ltimes \mathbb{R}^4$  as

$$\begin{aligned} \Phi' &= g \cdot \Phi \\ &= \begin{bmatrix} \Lambda^\mu{}_\nu & \mathbf{0} \\ \varphi_\nu & 1 \end{bmatrix} \cdot \begin{bmatrix} \pi^\nu \\ \phi \end{bmatrix} = \begin{bmatrix} \Lambda^\mu{}_\nu \pi^\nu \\ \phi + \varphi_\nu \pi^\nu \end{bmatrix}. \end{aligned} \tag{1.2}$$

As a result, the 5-vector representation can be viewed as a transpose of the Bargmann representation [51] of spacetime transformations, defined as  $\begin{bmatrix} x^{\mu'} \\ 1 \end{bmatrix} = \begin{bmatrix} \Lambda^\mu{}_\nu & \varphi^\mu \\ \mathbf{0} & 1 \end{bmatrix} \cdot \begin{bmatrix} x^\nu \\ 1 \end{bmatrix} = \begin{bmatrix} \Lambda^\mu{}_\nu x^\nu + \varphi^\mu \\ 1 \end{bmatrix}$ .

The appendix explores a sensible definition of dynamics for the 5-vector. Although a Poincaré-invariant Lagrangian can be constructed for this matter field [47, 48], its excessive degeneracy frustrates any causal link between its Poincaré symmetries and

conservation laws. In the appendix, another attempt to define dynamics for the 5-vector is pursued instead, employing a discrete Yang-Mills-type equation, called a  $\mathbb{1}$ -loop [49]. In this formulation of dynamics, a Poincaré Lie-algebra-valued matter current is defined on lattice links using neighboring 5-vector matter fields, as follows:

$$J_a[\mathbf{n}] = \left[ \Phi(\Phi_a^+)^T - \Phi_a^+ \Phi^T \right] \cdot \eta_0 \quad (1.3)$$

where  $\Phi = \Phi[\mathbf{n}]$ ,  $\Phi_a^+ = U_a[\mathbf{n}]^{-1} \Phi[\mathbf{n} + \hat{a}]$ , and  $\eta_0 = \mathbf{diag}(-1, 1, 1, 1, 0)$ . Here,  $J_a[\mathbf{n}]$  and  $U_a[\mathbf{n}]$  denote the current and Poincaré connection on the lattice edge  $[\mathbf{n}, \mathbf{n} + \hat{a}]$ . It is readily seen that  $J_a[\mathbf{n}]$  transforms in the adjoint representation, such that it can be readily paired with Wilson loops of gauge fields that transform in the same representation. Nevertheless, despite this progress, it will be unclear how to self-consistently define dynamics in  $\mathbb{1}$ -loop theory.

As a more practical consequence of this investigation, a Lorentz-invariant discretization of the tetradic Palatini action for general relativity is defined using a Poincaré gauge field. A structure-preserving variational algorithm is derived from this action by calculating its equations of motion for a gravitational field evolving in vacuum.

### 1.3 Organization

The remainder of this dissertation is structured as follows:

- **Chapter 2** reviews the pure mathematics necessary for the remaining chapters, with special attention to differential geometry and some background on Lie groups and Lie algebras;
- **Chapter 3** reviews elements of mathematical physics in the Hamiltonian and Lagrangian formalisms that assist in exploring the gauge structure of such sys-

tems;

- **Chapter 4** includes both review and original contributions, describing elements of structure-preserving algorithms that facilitate their preservation of gauge structure;
- **Chapter 5**, which is largely comprised of original contributions, synthesizes the development of the prior chapters to (i) study the gauge structure of existing plasma physics algorithms, as well as (ii) develop new gauge-structure-preserving algorithms.
- **The appendix** pursues a sensible discrete dynamical field theory for finite-dimensional Poincaré representations.

# 2

## Geometry and Symmetry I: Mathematical Preliminaries

In this chapter, relevant mathematical background is reviewed, drawing especially upon [34, 43, 52–56]. No claim of originality is made.

### 2.1 Manifolds and their pointwise structures

#### 2.1.1 Topological manifolds

Manifolds are objects that locally appear as if subsets of  $n$ -dimensional Euclidean space,  $\mathbb{R}^n$ . To make such an idea precise, an  *$n$ -dimensional topological manifold* is defined as a set  $M$  equipped with a countable *atlas*  $\mathcal{A} = \{(U_\alpha, \chi_\alpha)\}$  whose elements, called *coordinate charts*, are pairs of

- subsets  $U_\alpha \subset M$  (labeled here by  $\alpha$ ); and
- one-to-one maps  $\chi_\alpha : U_\alpha \rightarrow \mathbb{R}^n$  called *coordinate maps* onto connected open subsets  $\chi_\alpha(U_\alpha) \subset \mathbb{R}^n$

such that  $\mathcal{A}$  satisfies:

- (a)  $\bigcup_{\alpha} U_{\alpha} = M$ , i.e. the coordinate charts of  $\mathcal{A}$  cover  $M$ ;
- (b) on overlap  $U_{\alpha\beta} = U_{\alpha} \cap U_{\beta}$ , the composite map  $\chi_{\beta} \circ \chi_{\alpha}^{-1} : \chi_{\alpha}(U_{\alpha\beta}) \rightarrow \chi_{\beta}(U_{\alpha\beta})$  is  $\forall \alpha, \beta$  a homeomorphism (a continuous function with continuous inverse) of subsets of  $\mathbb{R}^n$ ; and
- (c)  $\forall$  distinct points  $m \in U_{\alpha}$  and  $m' \in U_{\beta} \exists$  open subsets  $V \subset \chi_{\alpha}(U_{\alpha})$  and  $V' \subset \chi_{\beta}(U_{\beta})$  in  $\mathbb{R}^n$  such that  $m \in \chi_{\alpha}^{-1}(V)$ ,  $m' \in \chi_{\beta}^{-1}(V')$ , and  $\chi_{\alpha}^{-1}(V) \cap \chi_{\beta}^{-1}(V') = \emptyset$ .

The dimension of  $M$  is denoted  $\mathbf{dim}M$ . The foregoing definition characterizes *topological* manifolds in that condition (b) requires the composite maps  $\chi_{\beta} \circ \chi_{\alpha}^{-1}$  (read “ $\chi_{\beta}$  after  $\chi_{\alpha}^{-1}$ ”) to be continuous, or  $C^0$ , between subsets of  $\mathbb{R}^n$ . The corresponding topology of  $M$  is generated by the preimages (under all  $\chi_{\alpha}$ ) of open sets in  $\mathbb{R}^n$ . Specifically, open sets on  $M$  are defined as any union of sets  $\{U = \chi_{\alpha}^{-1}(V) \mid V \subset \chi_{\alpha}(U_{\alpha}) \subset \mathbb{R}^n \text{ open}\}$ . With such a topology, the technical condition (c) enforces the Hausdorff separation axiom, which ensures that any two distinct points can be separated within disjoint open sets.  $\mathcal{A}$  can always be extended to a *maximal atlas*, so that it contains all possible coordinate charts that are compatible with  $\mathcal{A}$ . In particular, it will always be assumed that a given manifold has no atlas  $\mathcal{B} \supsetneq \mathcal{A}$  exists satisfying conditions (a)-(c).

It is often more useful to treat a manifold in local coordinates, that is, in terms of a particular coordinate chart near a point. For example, given a coordinate chart  $(U \ni m, x : U \rightarrow \mathbb{R}^n)$ , the point  $m$  might be more usefully described as the  $n$ -tuple  $x(m) = (x^1(m), \dots, x^n(m))$ . Similarly, a function on  $M$  is often treated in local coordinates as

$$f(m) = (f \circ x^{-1})(x(m)), \text{ and denoted as simply } f(x). \quad (2.1)$$

The ‘manifold philosophy’ holds that, despite the technical convenience of describing

a manifold  $M$  in terms of such local coordinates, as a geometric object  $M$  is unaffected by the coordinate choice; all coordinatizations by compatible charts are equally valid in any calculation of interest.

### 2.1.2 Smooth manifolds

A topological manifold is moreover a *smooth manifold*, or equivalently a *differentiable manifold*, if its composite maps  $\chi_\beta \circ \chi_\alpha^{-1}$  are not only  $C^0$ , but  $C^{k>0}$ —that is,  $k > 0$  times differentiable on  $\mathbb{R}^n$ . In fact, *smooth* will always be assumed to mean infinitely differentiable, so that smooth manifolds will have  $C^\infty$  composite maps.

As a trivial example, the Euclidean space  $\mathbb{R}^n$  is an  $n$ -dimensional smooth manifold for any  $n \in \mathbb{N}$ , coverable by a single coordinate chart defined by the identity map. Less trivially, the unit sphere  $S^2 = \{x \in \mathbb{R}^3 \mid |x| = 1\}$  is a two-dimensional smooth manifold that can be covered with the two coordinate charts

- stereographic projection from north pole:  $\chi_1(x, y, z) \Big|_{z < \epsilon} = \left(\frac{x}{1-z}, \frac{y}{1-z}\right)$
- stereographic projection from the south pole:  $\chi_2(x, y, z) \Big|_{z > -\epsilon} = \left(\frac{x}{1+z}, \frac{y}{1+z}\right)$

for any fixed  $0 < \epsilon < 1$ . The  $C^\infty$  composite map  $\chi_2 \circ \chi_1^{-1}$  is defined on the annular region  $\{(X, Y) \mid \frac{1-\epsilon}{1+\epsilon} < X^2 + Y^2 < \frac{1+\epsilon}{1-\epsilon}\} \subset \mathbb{R}^2$  and given by

$$\chi_2 \circ \chi_1^{-1}(X, Y) = \left(\frac{X}{X^2 + Y^2}, \frac{Y}{X^2 + Y^2}\right). \quad (2.2)$$

It will also be crucial to characterize maps between smooth manifolds. In particular, a map  $\phi : M \rightarrow M'$  is said to be *smooth* if  $\chi_{\beta'} \circ \phi \circ \chi_\alpha^{-1} : \mathbb{R}^n \rightarrow \mathbb{R}^{n'}$  is smooth wherever it is defined for any coordinate map  $\chi_\alpha$  on  $M$  and  $\chi_{\beta'}$  on  $M'$ . In this way, the smoothness of functions on manifolds is imputed from the familiar analysis of smooth functions on Euclidean space. Two smooth manifolds are said to be *diffeomorphic* if there exists a smooth map between them with smooth inverse, i.e., a *diffeomorphism*.

The set of infinitely differentiable functions between smooth manifolds  $M$  and  $N$  is denoted

$$C^\infty(M; N) = \{f : M \rightarrow N \mid f \text{ smooth}\}. \quad (2.3)$$

When  $N = \mathbb{R}$ ,  $C^\infty(M; N)$  is abbreviated as simply  $C^\infty(M)$ .

To better characterize the differential structure of manifolds, some useful definitions of algebraic objects are now presented.

### 2.1.3 An aside on algebraic spaces

#### Fields, vectors spaces, and tensor spaces

A *field*  $(K, +, \cdot)$  is a set  $K$  with addition and multiplication operations,

$$\begin{aligned} + : K \times K &\rightarrow K \quad \text{satisfying} \quad \{C^+ A^+ N^+ I^+\} \\ \cdot : K \times K &\rightarrow K \quad \text{satisfying} \quad \{C^+ A^+ N^+ (I)^+ \mid D^+\}, \end{aligned} \quad (2.4)$$

where  $CANI$  denotes commutativity, associativity, the existence of a neutral element, and inverses,  $D^+$  denotes distributivity, and  $(I)^+$  is in parentheses because only  $K/\{0\}$  is invertible. Examples of  $K$  include the rational, real, and complex numbers, respectively,  $\mathbb{Q}$ ,  $\mathbb{R}$ , and  $\mathbb{C}$ .

A *vector space*  $(V, \oplus, \odot|K)$  over a field  $(K, +, \cdot)$  is a set  $V$  with addition and multiplication operations,

$$\begin{aligned} \oplus : V \times V &\rightarrow V \quad \text{satisfying} \quad \{C^\oplus A^\oplus N^\oplus I^\oplus\} \\ \odot : K \times V &\rightarrow V \quad \text{satisfying} \quad \{A^\odot N^\odot \mid D^{+\odot} D^{\oplus\odot}\}, \end{aligned} \quad (2.5)$$

with distributivity over both  $+$  in  $K$  and  $\oplus$  in  $V$ .  $\odot$  may be referred to as *s-multiplication*. A *vector subspace* of  $V$  is any vector space  $U \subset V$  with operations

$(\oplus, \odot)$  inherited from  $V$ . A canonical example of a real vector space (over  $\mathbb{R}$ ) is the Euclidean space  $\mathbb{R}^n$ , whose operations are induced by addition and multiplication on  $\mathbb{R}$ . Similarly, any field is itself a one-dimensional vector space. In general, addition will be denoted on a vector space simply by  $+$  and any symbol for  $s$ -multiplication will simply be omitted.

A subset  $E \subset V$  of a vector space  $(V, +, \cdot | K)$  is called a (*Hamel*) *basis* of  $V$  if

- every finite subset  $\{e_1, \dots, e_n\} \subset E$  is linearly independent  
 (i.e.,  $\sum_{i=1}^n \alpha_i e_i = 0 \Rightarrow \alpha_i = 0$ ); and
- $\forall v \in V, \exists \alpha_i \in K, e_i \in E$  and  $n < \infty$  such that  $v = \sum_{i=1}^n \alpha_i e_i$ .

The second condition is also denoted  $\mathbf{span}(E) = V$ . (As an illustrative example, note that Fourier series do not form a Hamel basis, but a *Schauder basis* because an arbitrary function generally requires an infinite expansion in a Fourier basis.) The dimension of  $V$  is defined by the cardinality of  $E$ , that is,  $\mathbf{dim}V = |E|$ , which may be infinite.

A *linear map*  $\ell : V \rightarrow W$  between vector spaces  $(V, \oplus, \odot)$  and  $(W, \boxplus, \boxdot)$  over  $K$  is any map satisfying

$$\begin{aligned} \ell(v \oplus v') &= \ell(v) \boxplus \ell(v') \\ \ell(\alpha \odot v) &= \alpha \boxdot \ell(v) \end{aligned} \tag{2.6}$$

$\forall \alpha \in K, v, v' \in V$ . The set of all linear maps between vector spaces  $V$  and  $W$  is denoted  $\mathbf{Hom}(V, W)$  and called the set of *vector space homomorphisms*. (Notably,  $\mathbf{Hom}(V, W)$  is itself a vector space when defined to inherit the vector space structure of  $W$ .) Any bijective linear map between vector spaces is a *vector space isomorphism*. In fact, finite-dimensional vector spaces  $V$  and  $W$  defined over the same field are isomorphic if and only if  $\mathbf{dim}V = \mathbf{dim}W$ . *Endomorphisms* and *automorphisms* may be further defined on  $V$  as  $\mathbf{End}(V) = \mathbf{Hom}(V, V)$  and

$\mathbf{Aut}(V) = \{f \in \mathbf{End}(V) \mid f \text{ invertible}\} \subset \mathbf{End}(V)$ , respectively.

The *dual vector space*  $V^*$  of  $(V, +, \cdot | K)$  is defined as  $V^* = \mathbf{Hom}(V, K)$ , the set of linear maps from  $V$  to  $K$ . When  $\mathbf{dim}V < \infty$ , it is straightforward to show that  $\mathbf{dim}V^* = \mathbf{dim}V$ , and therefore  $V \cong V^*$  (where  $\cong$  indicates a vector space isomorphism). In particular, given a basis  $\{e_1, \dots, e_n\}$  of  $V$  with  $n < \infty$ , a *dual basis*  $\{\epsilon^1, \dots, \epsilon^n\} \subset V^*$  is defined on  $V^*$  such that

$$\epsilon^i(e_j) = \delta_j^i \quad \forall \quad 1 \leq i, j \leq n. \quad (2.7)$$

Likewise, it is readily seen that the dual of the dual satisfies  $V^{**} = \mathbf{Hom}(V^*, K) \cong V$ .

The vector space  $V$  and its dual  $V^*$  may be generalized as linear,  $K$ -valued maps defined with one another as domains. In particular, a  $(p, q)$  *tensor*  $T$  is defined as any multilinear map

$$T : \underbrace{V^* \times \dots \times V^*}_p \times \underbrace{V \times \dots \times V}_q \rightarrow K, \quad (2.8)$$

also denoted  $T : (V^*)^{\times p} \times V^{\times q} \rightarrow K$ . The  $(p, q)$  *tensor space*

$$T_q^p V = V^{\otimes p} \otimes (V^*)^{\otimes q} = \underbrace{V \otimes \dots \otimes V}_p \otimes \underbrace{V^* \otimes \dots \otimes V^*}_q = \{T \mid T \text{ is a } (p, q) \text{ tensor}\} \quad (2.9)$$

may then be defined as the set of all  $(p, q)$  multilinear maps. Here,  $\otimes$  denotes the *tensor product*, which takes arbitrary  $S \in T_q^p V$ ,  $S' \in T_s^r V$ , and defines  $S \otimes S' \in T_{q+s}^{p+r} V$  as the tensor that evaluates in order the correct number of vectors and dual vectors using  $S$  and  $S'$ , and multiplies the result over  $K$ . When  $T_q^p V$  inherits addition and

$s$ -multiplication operations from  $K$ ,  $(T_q^p V, \diamond, \diamond | K)$  constitutes a vector space:

$$\begin{aligned} \diamond : T_q^p V \times T_q^p V &\rightarrow T_q^p V \\ \diamond : K \times T_q^p V &\rightarrow T_q^p V. \end{aligned} \tag{2.10}$$

Notably,  $T_0^1 V = V$ ,  $T_1^0 V = V^*$ , and  $T_1^1 V \cong \mathbf{End} V$  are isomorphic vector spaces.  $(p, q)$  is also referred to as the *degree* of a tensor  $T \in T_q^p V$ . A tensor  $T \in T_q^0 V$  will also be called a  $q$ -linear map on  $V$ .

Given a basis  $\{e_1, \dots, e_{\mathbf{dim} V}\}$  of  $V$  and the dual basis  $\{\epsilon^1, \dots, \epsilon^{\mathbf{dim} V}\}$  of  $V^*$ , any tensor  $T \in T_q^p V$  can be specified by its components in these bases. In particular, one may fix  $T^{a_1 \dots a_p}_{b_1 \dots b_q} \in K$  for all indices  $1 \leq a_i, b_j \leq \mathbf{dim} V$ . The tensor  $T$  is then entirely determined by  $s$ -multiplication:

$$\begin{aligned} T &= \sum_{a_i=1}^{\mathbf{dim} V} \sum_{b_j=1}^{\mathbf{dim} V} T^{a_1 \dots a_p}_{b_1 \dots b_q} \diamond (e_{a_1} \otimes \dots \otimes e_{a_p} \otimes \epsilon^{b_1} \otimes \dots \otimes \epsilon^{b_q}) \\ &= T^{a_1 \dots a_p}_{b_1 \dots b_q} \diamond (e_{a_1} \otimes \dots \otimes e_{a_p} \otimes \epsilon^{b_1} \otimes \dots \otimes \epsilon^{b_q}). \end{aligned} \tag{2.11}$$

Here, the second equality may be taken to define Einstein summation convention.

## Rings, modules, and algebras

A *ring*  $(R, +, \cdot)$  is a set  $R$  with with addition and multiplication operations,

$$\begin{aligned} + : R \times R &\rightarrow R \quad \text{satisfying} \quad \{C^+ A^+ N^+ I^+\} \\ \cdot : R \times R &\rightarrow R \quad \text{satisfying} \quad \{A \mid D^+\}, \end{aligned} \tag{2.12}$$

however only *commutative unital rings* will be encountered, which satisfy  $\{C \cdot A \cdot N \mid D^+\}$ . Examples of  $R$  include the integers and smooth functions on a manifold  $M$ , respectively,  $\mathbb{Z}$  and  $C^\infty(M)$ . A ring generalizes the notion of a field; in particular, a field is a *commutative division ring*.

A *left R-module*  $(M_R, \oplus, \odot)$  over a ring  $(R, +, \cdot)$  is a set  $M_R$  with addition and multiplication operations,

$$\begin{aligned} \oplus : M_R \times M_R &\rightarrow M_R \quad \text{satisfying} \quad \{C^\oplus A^\oplus N^\oplus I^\oplus\} \\ \odot : R \times M_R &\rightarrow M_R \quad \text{satisfying} \quad \{A^\odot N^\odot \mid D^{+\odot} D^{\oplus\odot}\}, \end{aligned} \tag{2.13}$$

with distributivity over both  $+$  in  $R$  and  $\oplus$  in  $M_R$ . A *right R-module* is correspondingly defined with a right multiplication operation  $\odot : M_R \times R \rightarrow M_R$  and an *R-bimodule* is defined with both left and right multiplications. A module generalizes the notion of a vector space; in particular, any vector space  $(V, \oplus, \odot \mid K)$  is a  $K$ -module over the field  $K$ .

An *algebra*  $(A, \oplus, \odot, \bullet \mid K)$  is a vector space  $A$  equipped with a bilinear map

$$\bullet : A \times A \rightarrow A. \tag{2.14}$$

As an example, note that  $C^\infty(M)$  can be equally well regarded as a ring or an associative algebra; it is a vector space over  $\mathbb{R}$  with the bilinear map of multiplication,  $(f \bullet g)(m) = f(m) \cdot g(m)$ . Another crucial example of an algebra is a Lie algebra, which has a non-associative multiplication rule  $\bullet$  denoted  $[\cdot, \cdot]$ , as shall be later described. A linear map  $D \in \mathbf{End}(A)$  from an algebra  $A$  to itself is called a *derivation* if  $D$  respects the Leibniz rule, that is,

$$D(f \bullet g) = D(f) \bullet g + f \bullet D(g). \tag{2.15}$$

Given these algebraic structures, differential structures can now be characterized on manifolds.

### 2.1.4 Tangent spaces

The differentiation of functions on  $M$  can be geometrically characterized in the following way. Consider a smooth curve  $\gamma : \mathbb{R} \rightarrow M$  through  $m \in M$ , parametrized (without loss of generality) so that  $\gamma(0) = m$ . The *directional derivative of  $f$  at  $m$  along  $\gamma$*  is defined as a linear map

$$X_{\gamma,m} : C^\infty(M) \rightarrow \mathbb{R} \quad (2.16)$$

$$f \mapsto (f \circ \gamma)'(0) = \left. \frac{d}{ds} \right|_{s=0} (f \circ \gamma).$$

$X_{\gamma,m}$  is called the *tangent vector* to  $\gamma$  at  $m$ . A precise intuition is that  $X_{\gamma,m}$  is the velocity of the curve  $\gamma$ .

The set of all tangent vectors at  $m$  forms a real vector space called the *tangent space of  $M$  at  $m$* , denoted

$$T_m M = \{X_{\gamma,m} \mid \gamma \text{ is a smooth curve through } m\}. \quad (2.17)$$

$T_m M$  is closed under addition and multiplication since, given paths  $\{\gamma, \delta\}$  such that  $\gamma(0) = \delta(0) = m \in U$ , for any chart  $(U, \chi)$  the path  $\sigma(s) = \chi^{-1} \circ (\chi \circ \gamma(as) + \chi \circ \delta(bs) - \chi(m))$  satisfies  $X_{\sigma,m} = aX_{\gamma,m} + bX_{\delta,m} \quad \forall a, b \in \mathbb{R}$ .

By considering the tangent vectors along curves determined by coordinate charts—namely, curves over which only one coordinate varies—it is straightforward to show that  $\mathbf{dim}(T_m M) = \mathbf{dim} M$ . In particular, consider a coordinate chart  $(U, x)$  with  $x : U \rightarrow \mathbb{R}^n$  such that  $x(m) = (x^1(m), \dots, x^n(m))$ , and a curve  $\gamma_i : \mathbb{R} \rightarrow U$  through  $m \in U$  such that  $\gamma_i(0) = m$  and  $x^j \circ \gamma_i(s) = s\delta_i^j$ . (Here,  $\delta_i^j$  is the Kronecker delta.)

The derivative of  $f \in C^\infty(M)$  along  $\gamma_i$  is then given by

$$\begin{aligned}
X_{\gamma_i, m}(f) &= (f \circ \gamma_i)'(0) = (f \circ x^{-1} \circ x \circ \gamma_i)'(0) \\
&= \partial_j (f \circ x^{-1}) \Big|_{x(\gamma_i(0))} (x^j \circ \gamma_i)'(0) \\
&= \partial_j (f \circ x^{-1}) \Big|_{x(m)} \delta_i^j \\
&= \partial_i (f \circ x^{-1}) \Big|_{x(m)} \\
&= \left( \frac{\partial}{\partial x^i} f \right) \Big|_m .
\end{aligned} \tag{2.18}$$

The second line follows from the chain rule on  $\mathbb{R}^n$  and the Einstein summation convention, where the symbol  $\partial_j$  denotes a derivative with respect to the  $j^{\text{th}}$  entry of the  $n$ -tuple  $(x^1, \dots, x^n)$  on  $\mathbb{R}^n$ . The last two lines define the *partial derivative* of  $f : M \rightarrow \mathbb{R}$ , which is always evaluated with respect to a particular coordinate chart on  $M$ .

Repeating the calculation of Eq. (2.18) for a general curve  $\gamma$ , note that

$$X_{\gamma, m}(f) = \frac{\partial f}{\partial x^i} \Big|_m (x^i \circ \gamma)'(0) = \left[ (x^i \circ \gamma)'(0) \frac{\partial}{\partial x^i} \Big|_m \right] f. \tag{2.19}$$

A tangent vector can thus be expanded in the partial derivatives of a local coordinate chart—

$$X_{\gamma, m} = X_{\gamma, m}^i \frac{\partial}{\partial x^i} \Big|_m \quad \text{where} \quad X_{\gamma, m}^i = (x^i \circ \gamma)'(0) \tag{2.20}$$

are its real coefficients (or *components*). The components of  $X_{\gamma, m}$  in a particular coordinate chart provide a means to describe a tangent vector independent of any fixed curve  $\gamma$ . From hereon, therefore, a tangent vector will be labeled simply by the

point at which it is ‘attached’, i.e.

$$X_m = X_m^i \frac{\partial}{\partial x^i} \Big|_m. \quad (2.21)$$

It is worth noting that such a vector can arise from infinitely many possible curves (namely, any curve with the correct first order Taylor expansion at  $m$ ). From this perspective,  $X_m$  is best viewed simply as a differential operator on smooth functions at  $m$ .

Eq. (2.21) makes clear that the partial derivatives of an arbitrary chart span  $T_m M$ . Their linear independence also follows from noting that  $\partial x^j / \partial x^i = \delta_i^j$  on each ‘coordinate function’  $x^j$  (defined such that  $x^j \circ x^{-1}$  is a projection map on  $\mathbb{R}^n$ ). Therefore,  $\{\partial_{x^i}\}$  forms a basis for  $T_m M$  and  $\mathbf{dim}(T_m M) = \mathbf{dim} M$  as desired.

A range of notations are used for the partial derivative, and hereafter it will be denoted by any of the following:

$$\frac{\partial f}{\partial x^i} = \partial_{x^i} f = \partial_i f = f_{,i}. \quad (2.22)$$

To transform a tangent vector expressed in a local coordinate basis  $\left\{ \frac{\partial}{\partial x^1}, \dots, \frac{\partial}{\partial x^n} \right\}$  to its expression in another coordinate basis  $\left\{ \frac{\partial}{\partial x^{1'}}, \dots, \frac{\partial}{\partial x^{n'}} \right\}$ , note by the chain rule that  $\frac{\partial}{\partial x^i} = \frac{\partial x^{j'}}{\partial x^i} \frac{\partial}{\partial x^{j'}}$ . Substituting into Eq. (2.21), therefore, the following transformation of the components of  $X_m$  is found:

$$X_m = X_m^i \frac{\partial}{\partial x^i} \Big|_m = \left( X_m^i \frac{\partial x^{j'}}{\partial x^i} \right) \frac{\partial}{\partial x^{j'}} \Big|_m \quad \text{i.e.,} \quad X_m^{j'} = X_m^i \frac{\partial x^{j'}}{\partial x^i}. \quad (2.23)$$

### 2.1.5 Cotangent and tensor spaces

Having seen that the tangent space  $T_m M$  defines a vector space, its dual may also be defined, the *cotangent space at  $m$* ,

$$T_m^* M = (T_m M)^*, \quad (2.24)$$

whose elements are called *covectors*. Just as the basis  $\{\frac{\partial}{\partial x^1}, \dots, \frac{\partial}{\partial x^n}\}$  for  $T_m M$  is determined by a local coordinate chart  $(U, x)$ , a dual basis  $\{dx^1, \dots, dx^n\}$  of  $T_m^* M$  can be constructed for the same chart, satisfying

$$dx^i \left( \frac{\partial}{\partial x^j} \right) = \delta_j^i \quad (2.25)$$

as in Eq. (2.7).

A covector must transform under coordinate transformations in a manner that preserves Eq. (2.25). This requires an ‘inversion’ of the vector transformation in Eq. (2.23), so that the components of a covector  $\alpha = \alpha_i dx^i$  transform into the basis  $\{dx^{i'}, \dots, dx^{n'}\}$  via

$$\alpha_{j'} = \alpha_i \frac{\partial x^i}{\partial x^{j'}}. \quad (2.26)$$

More generally, the  $(p, q)$  *tensor space at  $m$*  may be defined as

$$\begin{aligned} T_m^{(p,q)} M &= T_q^p(T_m M) \\ &= \{T : (T_m^* M)^{\times p} \times (T_m M)^{\times q} \rightarrow \mathbb{R} \mid T \text{ multilinear} \} \end{aligned} \quad (2.27)$$

whose generic element can be expressed in a local coordinate basis as

$$T = T^{a_1 \dots a_p}_{b_1 \dots b_q} \left( \frac{\partial}{\partial x^{a_1}} \otimes \dots \otimes \frac{\partial}{\partial x^{a_p}} \otimes dx^{b_1} \otimes \dots \otimes dx^{b_q} \right). \quad (2.28)$$

as in Eq. (2.11). Since each (vector and covector) component of the tensor must transform in keeping with Eqs. (2.23) and (2.26), it follows that

$$T_{b'_1 \dots b'_q}^{a'_1 \dots a'_p} = T_{b_1 \dots b_q}^{a_1 \dots a_p} \frac{\partial x^{a'_1}}{\partial x^{a_1}} \cdots \frac{\partial x^{a'_p}}{\partial x^{a_p}} \frac{\partial x^{b_1}}{\partial x^{b'_1}} \cdots \frac{\partial x^{b_q}}{\partial x^{b'_q}} \quad (2.29)$$

Evidently,  $T_m^{(0,0)} M = \mathbb{R}$ ,  $T_m^{(1,0)} M = T_m M$  and  $T_m^{(0,1)} M = T_m^* M$ .

## 2.2 Manifolds and their global structures

Thus far, tangent, cotangent, and tensor spaces have been described as independent algebraic objects ‘attached’ at a given point of a manifold  $M$ . Since such objects ultimately arise from the infinitesimal characterization of curves traversing a continuum of points on  $M$ , however, it would seem natural to describe these spaces in a manner that is more geometrically unified. Doing so begins to reveal the rich structure of smooth manifolds.

### 2.2.1 Submanifolds and product manifolds

A *submanifold* is a subset  $N \subset M$  that is itself a manifold, whose manifold structure is inherited from  $M$ . In particular, one requires that  $\forall m \in N, \exists$  a chart  $(U_\alpha, \chi_\alpha)$  on  $M$  such that  $m \in U_\alpha$  and  $\chi_\alpha(N \cap U_\alpha) = \mathbb{R}^{\dim N} \cap \chi_\alpha(U_\alpha)$  for  $\mathbb{R}^{\dim N} \subseteq \mathbb{R}^{\dim M}$ .

This condition can be equivalently stated by requiring  $N \subset M$  to be the image of a *maximal rank* map into  $M$ . In particular, the *rank* at  $x \in Q$  of an arbitrary smooth map  $F : Q \rightarrow P$  between the  $q$ -dimensional manifold  $Q$  and  $p$ -dimensional manifold  $P$ —denoted  $\mathbf{rank}(F)_x$ —is the rank of the  $q \times p$  *Jacobian matrix*  $\left. \frac{\partial F^j}{\partial x^i} \right|_x$ . (Here, the notation of Eq. (2.1) for arbitrary coordinate charts  $x^i$  on  $Q$  and  $y^j = F^j(x)$  on  $P$  is used.)  $\mathbf{rank}(F)_x$  is said to be *maximal* if  $\mathbf{rank}(F)_x = \mathbf{min}(q, p)$ , its greatest attainable value. By the implicit function theorem, given any maximal rank  $F$ , coordinates can always be chosen such that  $y = F(x) = (x^1, \dots, x^q, 0, \dots, 0)$  if  $p > q$

or  $y = F(x) = (x^1, \dots, x^q)$  if  $p \leq q$ . Therefore, given  $N$  as the image of a maximal rank map  $\phi : N_0 \rightarrow N \subset M$  for some smooth manifold  $N_0$ , a coordinate chart can be defined satisfying the definition of submanifold above.

In the other direction, there is often occasion to ‘augment’ manifolds via the natural structure of a *product manifold*. In particular, the product of an  $n$ -dimensional manifold  $M$  and an  $n'$ -dimensional manifold  $M'$  is defined by the manifold  $M \times M' = \{(m, m') \mid m \in M, m' \in M'\}$ . Its coordinate maps are defined such that, given  $\chi_\alpha(m) = (\chi_\alpha^1(m), \dots, \chi_\alpha^n(m)) \in \mathbb{R}^n$  on  $U_\alpha \subset M$  and  $\chi_{\beta'}(m') = (\chi_{\beta'}^1(m'), \dots, \chi_{\beta'}^{n'}(m')) \in \mathbb{R}^{n'}$  on  $U_{\beta'} \subset M'$ , the product manifold has coordinate map  $\chi_{\alpha \times \beta'}((m, m')) = (\chi_\alpha^1(m), \dots, \chi_\alpha^n(m), \chi_{\beta'}^1(m'), \dots, \chi_{\beta'}^{n'}(m')) \in \mathbb{R}^{n+n'}$  on  $U_\alpha \times U_{\beta'} \subset M \times M'$ . Therefore,  $\mathbf{dim}(M \times M') = n + n'$ .

## 2.2.2 Fiber bundles over smooth manifolds

A *fiber bundle* with fiber  $F$  over a smooth manifold  $M$  is denoted  $E \xrightarrow{\pi} M$ , where  $E$  is a smooth manifold called the *total space*,  $M$  is the *base manifold* or *base space*, and  $\pi : E \rightarrow M$  is a smooth surjective map called the *projection* that satisfies a *local triviality* property with respect to the smooth manifold  $F$ . This property requires that  $\forall m \in M$ , there exists a neighborhood  $U \subset M$  containing  $m$  such that  $\pi^{-1}(U) \cong_{\text{diff}} U \times F$  are diffeomorphic. A fiber bundle can therefore be imagined as a set of spaces diffeomorphic to  $F$ , smoothly parametrized by the points of  $M$ . The preimage  $\pi^{-1}(m) \subset E$  of a point in  $M$  is called the *fiber at  $m$* , and satisfies  $\pi^{-1}(m) \cong_{\text{diff}} F$ .

A smooth map  $\sigma : M \rightarrow E$  is called a *section* of the fiber bundle  $E$  if  $\pi \circ \sigma = \mathbf{id}_M$ , the identity map on  $M$ . A section can therefore be understood as a map from each point  $m \in M$  ‘‘up’’ to a point in  $\pi^{-1}(m)$ , the fiber above  $m$ . The set of all sections of a fiber bundle  $E$  will be denoted  $\Gamma(E)$ . A *local section* is a smooth map  $\sigma_{\text{loc}} : U \rightarrow E$  from any open set  $U \subset M$  satisfying  $\pi|_U \circ \sigma_{\text{loc}} = \mathbf{id}_U$ . The set of all local sections of

a bundle  $E$  will be denoted  $\Gamma_{\text{loc}}(E)$ .

If there exist smooth maps  $u : E \rightarrow E'$  and  $f : M \rightarrow M'$  between the fiber bundles  $E \xrightarrow{\pi} M$  and  $E' \xrightarrow{\pi'} M'$  such that  $\pi' \circ u = f \circ \pi$ , then  $(u, f)$  is said to be a *bundle map*. (Note that  $f$  is in fact uniquely determined by  $u$ .) If  $u$  and  $f$  have smooth inverses as well, then  $(u, f)$  defines a *bundle isomorphism*. A *subbundle*  $E' \xrightarrow{\pi'} M'$  is defined such that  $E' \subset E$  and  $M' \subset M$  are submanifolds and  $\pi' = \pi|_{E'}$  is given by the restriction of the projection map on  $E$ .

The simplest example of a fiber bundle is a product space  $E = M \times F$  for some manifold  $F$ , where  $\pi(m, f) = m$ . Any fiber bundle that is bundle isomorphic to a product space is called a *trivial bundle*. The *local trivialization* of a fiber bundle with fibers diffeomorphic to  $F$  is given by a product  $U \times F$  such that  $U \times F \cong_{\text{diff}} \pi^{-1}(U)$  for any open  $U \subset M$ . On any such trivialization, a local section  $\sigma_{\text{loc}}(U)$  can always be defined.

A typical example of a nontrivial fiber bundle is the Moebius strip, with a base space defined by the circle  $S^1$  and a fiber defined by the interval  $[0, 1] \subset \mathbb{R}$ . The requirement of the projection map's continuity forces  $\pi$  to continuously 'twist' as it traverses through fibers above the base space, which distinguishes the Moebius strip from the cylinder,  $S^1 \times [0, 1]$ .

### 2.2.3 Tangent bundles

Certain bundles on manifolds will be of particular interest. Foremost is the collection of all tangent spaces on  $M$ , defined as the *tangent bundle*

$$TM = \bigcup_{m \in M} T_m M, \quad (2.30)$$

whose bundle projection is  $TM \xrightarrow{\pi} M$ , and whose fibers are given by  $\pi^{-1}(m) = T_m M$ . It is worth noting that vectors in two different tangent spaces belong to separate

algebraic entities and cannot be added together, so that  $X_m + X_{m'}$  is ill-defined for  $m \neq m' \in M$ .

$TM$  is itself a manifold, whose atlas can be inherited from the  $n$ -dimensional base space  $M$  by associating to each chart  $(U, x)$  on  $M$  a chart  $(\pi^{-1}(U), \xi)$  on  $TM$ , defined such that  $\xi(X_m) = (x^1(m), \dots, x^n(m), X_m^1, \dots, X_m^n) \in \mathbb{R}^{2n}$ . Here,  $X_m = X_m^i \partial_i \in T_m M$  with components determined by the chart as described in Eq. (2.21). Clearly,  $\mathbf{dim}(TM) = 2n$ . Given a smooth manifold  $M$ ,  $TM$  is also smooth and the projection  $\pi : TM \rightarrow M$  is a smooth map.

## 2.2.4 Vector fields

The crucial notion of a *vector field* on a manifold  $M$  is now straightforwardly described. In particular, a vector field is any smooth section  $\sigma : M \rightarrow TM$  of the tangent bundle. The set of all vector fields (i.e. all smooth sections) is denoted  $\mathfrak{X}(M)$  (equivalently,  $\Gamma(TM)$ ).

It is clear that a vector field is smooth if and only if its coefficient functions in local coordinates are smooth. In other words, a vector field is locally defined by  $X = X^i(x) \partial_{x^i}$  for some  $\{X^i(x) \in C^\infty(M)\}$ . It thus follows that  $\mathfrak{X}(M)$  forms a module over the ring  $C^\infty(M)$ , so that vector fields may be added and multiplied by smooth functions, e.g. for  $f, g \in C^\infty(M)$  and  $X, Y \in \mathfrak{X}(M)$ ,  $fX + gY$  defines another vector field in  $\mathfrak{X}(M)$ , where  $fX = f(x)X^i(x)\partial_i$ . (Note, however, that vector fields need not have components that are well-defined globally, since coordinate charts need not cover an entire manifold. Nevertheless,  $\{\partial_{x^i}\}$  constitutes a bona fide basis on a local coordinate chart  $(U, x)$  for the  $C^\infty(M)$ -module  $\mathfrak{X}(U \subset M)$ .)

In local coordinates, it can also be shown that, given any  $f \in C^\infty(M)$  and  $X \in \mathfrak{X}(M)$  it follows that  $X(f) \in C^\infty(M)$ , where  $X(f)$  denotes the directional derivative described in Section 2.1.4. (The curve locally associated with a vector field will be described in the next section.) By the addition and product rules, in fact, any

vector field  $X \in \mathfrak{X}(M)$  is a derivation on the algebra  $C^\infty(M)$ ; it acts linearly and respects the Leibniz rule of Eq. (2.15). Therefore,

$$X(fg) = X(f)g + fX(g) \quad \forall f, g \in C^\infty(M) \text{ and } X \in \mathfrak{X}(M). \quad (2.31)$$

Powerfully, it also turns out that any derivation on  $C^\infty(M)$  is a vector field. This can be seen by examining the derivation operating on coordinate functions. In particular, for an arbitrary derivation  $D : C^\infty(M) \rightarrow C^\infty(M)$ , define  $D(x^i) = a^i(x)$  in local coordinates. By Taylor's theorem, near a point  $x_0$  an arbitrary  $f \in C^\infty(M)$  can be written as  $f(x) = f(x_0) + (x^i - x_0^i)h_i(x)$  for some functions  $\{h_i \in C^\infty(M)\}$  satisfying  $h_i(x_0) = \frac{\partial f}{\partial x^i} \Big|_{x_0}$ . Since  $D(c) = 0 \quad \forall c \in \mathbb{R}$ , it follows that  $Df(x) = a^i(x)h_i(x) + (x^i - x_0^i)Dh_i(x)$ . Letting  $x \rightarrow x_0$  establishes  $D = a^i(x)\frac{\partial}{\partial x^i}$ .

## 2.2.5 Flows of vector fields

In Eq. (2.16), a curve  $\gamma$  was demonstrated to give rise to a tangent vector  $X_{\gamma, m}$  at each point  $m \in \mathbf{Im}\gamma$  (where  $\mathbf{Im}\gamma$  denotes the image of  $\gamma$ ). With individual tangent vectors comprising a smooth vector field on  $M$ , this process can be run in reverse, so that tangent vectors give rise to a curve. In particular, an *integral curve* of a vector field  $X \in \mathfrak{X}(M)$  is a smooth curve  $\gamma : \mathbb{R} \rightarrow M$  whose tangent vector equals the vector field at each point along  $\gamma$ .

In local coordinates, the integral curve arises by Eq. (2.20) as the solution  $x(s) = (x^1(s), \dots, x^n(s))$  to the ordinary differential equations (ODEs)

$$\frac{dx^i}{ds} = X^i(x) \quad \forall i \in \{1, \dots, n\} \quad (2.32)$$

where  $X = X^i(x)\partial_{x^i} \in \mathfrak{X}(M)$ . (Here, the notation of Eq. (2.1) is employed.) Given any initial condition  $x(0)$ , existence and uniqueness theorems of ODEs ensure that there is a unique solution to Eq. (2.32), that is, an integral curve for  $X$ , in some

neighborhood of  $x(0)$ . This implies, in turn, the existence of a unique *maximal integral curve* of  $X$  initialized at any  $x(0)$  and integrated to maximal  $s$  (such that  $s \rightarrow \infty$  if no divergence or boundary is reached in ‘finite time’).

The parametrized maximal integral curve of  $X$  passing through  $m \in M$  can also be regarded as a function of the initial point  $m = x(0)$  and denoted  $\Psi_s(m) = x(s)$ . When the ‘existence time’ is infinite for all maximal integral curves of  $X$ ,  $\Psi_s : M \rightarrow M$  defines a diffeomorphism  $\forall s \in \mathbb{R}$ , and the set  $\{\Psi_s : M \rightarrow M\}_{s \in \mathbb{R}}$  defines a one-parameter family of diffeomorphisms on  $M$  called the *flow generated by  $X$* . From the uniqueness of solutions to Eq. (2.32), it is clear that  $\Psi_s$  satisfies

$$\begin{aligned}\Psi_{s'}(\Psi_s(m)) &= \Psi_{s+s'}(m) \\ \Psi_0(m) &= m \\ \frac{d\Psi_s(m)}{ds} &= X_{\Psi_s(m)}.\end{aligned}\tag{2.33}$$

Flows are also invertible, since  $\Psi_s \circ \Psi_{-s} = \mathbf{id}_M$ .

Another quite useful notation for the flow of a vector field  $X$  is given by

$$\exp(sX)m = \Psi_s(m),\tag{2.34}$$

in which the vector field  $X$  is imagined to ‘act on’ the point  $m$ . This notation is justified by noting that Eq. (2.33) results in

$$\begin{aligned}\exp(s'X)\exp(sX)m &= \exp((s+s')X)m \\ \exp(0X)m &= m \\ \frac{d}{ds}\exp(sX)m &= X_{\exp(sX)m}\end{aligned}\tag{2.35}$$

—properties characteristic of the exponential.

## 2.2.6 Pushforward

Vector fields behave naturally with respect to maps between smooth manifolds. Given a vector field  $X \in \mathfrak{X}(M)$  and a smooth map  $f : M \rightarrow N$  such that  $f(m) = n$ , the *pushforward of  $X$  at  $m \in M$*  is defined as the map

$$\begin{aligned} f_* : T_m M &\rightarrow T_n N \\ X_m &\mapsto Y_n \quad \text{s.t.} \quad (f_* X_m)(h) = Y_n(h) = X_m(h \circ f) \quad \forall h \in C^\infty(N). \end{aligned} \tag{2.36}$$

(Note that Eq. (2.16) therefore defines  $X_{\gamma, m} = \gamma_* \frac{d}{ds}$  for the vector field  $\frac{d}{ds} \in T\mathbb{R}$ .) In local coordinates  $(U, x)$  on  $M$  and  $(V, y)$  on  $N$ , the pushforward of  $X_m$  is given by

$$Y_n = f_* X_m = X_m(f^j) \frac{\partial}{\partial y^j} \Big|_n = X_m^i \frac{\partial f^j}{\partial x^i} \frac{\partial}{\partial y^j} \Big|_n. \tag{2.37}$$

The pushforward transforms  $X_m$  simply by a factor of the Jacobian matrix  $\partial f^j / \partial x^i$ , a generalized first derivative of maps between manifolds.  $f_*$  is clearly, therefore, linear.

From the definition, it is immediate to see that pushforwards are covariant, that is,

$$(f \circ g)_* = f_* \circ g_* \tag{2.38}$$

—which constitutes a reformulation of the chain rule. If  $f$  is not just smooth but a diffeomorphism, then  $f_* : \mathfrak{X}(M) \rightarrow \mathfrak{X}(N)$  maps vector fields on  $M$  to vector fields on  $N$  (and not just individual vectors).

The pushforward  $f_*$  is also sometimes referred to as the *differential*, denoted  $df$ , or the tangent map, denoted  $Tf$ .

### 2.2.7 The Jacobi-Lie bracket

The differential structure of manifolds is further revealed by a crucial operation on its vector fields known as the *Jacobi-Lie bracket*, or the *vector field commutator*. Given two vector fields  $X, Y \in \mathfrak{X}(M)$ , their Jacobi-Lie bracket  $[X, Y] \in \mathfrak{X}(M)$  is another vector field, defined such that

$$[X, Y](f) = X(Y(f)) - Y(X(f)) \quad (2.39)$$

$\forall f \in C^\infty(M)$ . In local coordinates  $(U, x)$  on  $M$ , it is straightforward to see that

$$[X, Y](x) = \left( X^j \frac{\partial Y^i}{\partial x^j} - Y^j \frac{\partial X^i}{\partial x^j} \right) \frac{\partial}{\partial x^i} \quad (2.40)$$

(and that second derivatives cancel out). Simply from the definition, it can be shown that the Lie bracket  $[\cdot, \cdot]$  satisfies three properties:

- (a) *Bilinearity.*  $[aX + bY, Z] = a[X, Z] + b[Y, Z]$   
 $[X, aY + bZ] = a[X, Y] + b[X, Z];$
- (b) *Skewness.*  $[X, Y] = -[Y, X];$  and the
- (c) *Jacobi Identity.*  $[X, [Y, Z]] + [Y, [Z, X]] + [Z, [X, Y]] = 0$

$\forall a, b \in \mathbb{R}$  and  $X, Y, Z \in \mathfrak{X}(M)$ .

Any algebra satisfying the three properties above is called a *Lie algebra*. Thus,  $\mathfrak{X}(M)$  constitutes an infinite-dimensional Lie algebra with a multiplication rule defined by the Jacobi-Lie bracket. Furthermore, by rewriting the Jacobi identity as  $[X, [Y, Z]] = [[X, Y], Z] + [Y, [X, Z]]$ , the Jacobi identity is seen equivalent to the requirement that the operator  $[X, \cdot] : \mathfrak{X}(M) \rightarrow \mathfrak{X}(M)$  is a derivation  $\forall X \in \mathfrak{X}(M)$ .

## 2.2.8 Cotangent and tensor bundles

A construction entirely analogous to the tangent bundle may be undertaken to define the *cotangent bundle*

$$T^*M = \bigcup_{m \in M} T_m^*M \quad (2.41)$$

whose smooth sections are *covector fields*, e.g.  $\alpha \in \Gamma(T^*M)$ . Like vector fields, covector fields may be expressed locally in a coordinate chart  $\alpha = \alpha_i(x)dx^i$ , where  $\alpha_i(x) \in C^\infty(M) \forall i \in \{1, \dots, \mathbf{dim}M\}$ .

Lastly, the more general  $(p, q)$  *tensor bundle* can be defined as

$$T^{(p,q)}M = \bigcup_{m \in M} T_m^{(p,q)}M, \quad (2.42)$$

whose smooth sections are *tensor fields*. Equivalently tensor fields on a smooth manifold  $M$  can be characterized as the set of  $C^\infty(M)$ -linear maps

$$T^{(p,q)}M = \{T : \Gamma(T^*M)^{\times p} \times \Gamma(TM)^{\times q} \rightarrow C^\infty(M) \mid T \text{ linear}\}. \quad (2.43)$$

Tensor fields, too, may be locally described in terms of a coordinate chart, e.g.  $T = T^{a_1 \dots a_p}_{b_1 \dots b_q}(x) \left( \frac{\partial}{\partial x^{a_1}} \otimes \dots \otimes \frac{\partial}{\partial x^{a_p}} \otimes dx^{b_1} \otimes \dots \otimes dx^{b_q} \right)$ , where  $T^{a_1 \dots a_p}_{b_1 \dots b_q}(x) \in C^\infty(M)$  are smooth, locally defined component functions.

Clearly,  $T^{(0,0)}M = C^\infty(M)$ ,  $T^{(1,0)}M = TM$  and  $T^{(0,1)}M = T^*M$ .

## 2.3 Exterior algebra, differential forms and de Rham cohomology

While covector fields have so far been discussed primarily as ancillary objects dual to vector fields, they play a much more essential role when generalized to the category

of differential forms.

### 2.3.1 Exterior algebra

To build up to a definition of differential forms, it is useful to first consider the algebraic notion of an *exterior algebra*. For any real vector space  $V$ , the space of  $k$ -linear maps  $T_k^0 V$  may be further specialized to  $\mathbf{Alt}^k V \subset T_k^0 V$ , the space of *alternating* ( $k \geq 0$ )-linear maps, defined as

$$\mathbf{Alt}^k V = \left\{ \omega \in T_k^0 V \mid \omega(X_1, \dots, X_k) = (-1)^{|\pi|} \omega(X_{\pi(1)}, \dots, X_{\pi(k)}) \quad \forall X_i \in V, \pi \in \mathbf{Perm}(k) \right\}, \quad (2.44)$$

where  $\mathbf{Perm}(k)$  denotes permutations on  $k$  elements and  $|\pi|$  denotes a permutation's parity. In short, any alternating  $k$ -linear map  $\omega \in \mathbf{Alt}^k V$  is antisymmetric in its inputs. For good measure, note that  $\mathbf{Alt}^0 V = T_0^0 V = \mathbb{R}$  and  $\mathbf{Alt}^1 V = T_1^0 V = V^*$ .

Given a basis  $(e_1, \dots, e_n)$  for  $V$ , it is apparent that the antisymmetric  $\omega \in \mathbf{Alt}^k V$  is entirely determined by its values  $\omega(e_{\sigma(1)}, \dots, e_{\sigma(k)})$  on basis elements represented by 'increasing maps'  $\sigma : \{1, \dots, k\} \rightarrow \{1, \dots, n\}$  satisfying  $\sigma(1) < \dots < \sigma(k)$ . The set of such increasing maps is denoted  $\vec{\Sigma}_k^n$ , a set of cardinality  $\#\vec{\Sigma}_k^n = \binom{n}{k}$ . The evaluations  $\left\{ \omega(e_{\sigma(1)}, \dots, e_{\sigma(k)}) \mid \sigma \in \vec{\Sigma}_k^n \right\}$  therefore define a basis for  $\mathbf{Alt}^k V$ , so that  $\mathbf{Alt}^k V$  is a vector space of dimension  $\binom{n}{k}$ —a significant reduction to the  $n^k$  dimensionality of  $T_k^0 V$ .

The antisymmetry of an alternating  $k$ -linear map manifests in the antisymmetry of its components, such that

$$\omega_{a_1 \dots a_k} = \omega_{[a_1 \dots a_k]} = \frac{1}{k!} \sum_{\pi \in \mathbf{Perm}(k)} (-1)^{|\pi|} \omega_{a_{\pi(1)} \dots a_{\pi(k)}}. \quad (2.45)$$

As defined here, square brackets around indices are used to denote antisymmetrization, while parentheses around indices would denote symmetrization (with a defining

formula as above, less the factor of  $(-1)^{|\pi|}$ .

The *wedge product*  $\omega \wedge \rho \in \mathbf{Alt}^{k+\ell}V$  may now be formulated for any  $\omega \in \mathbf{Alt}^kV$  and  $\rho \in \mathbf{Alt}^\ell V$ . It is defined such that

$$\begin{aligned} (\omega \wedge \rho)(X_1, \dots, X_{k+\ell}) &= \frac{1}{k!\ell!} \sum_{\pi \in \mathbf{Perm}(k+\ell)} (-1)^{|\pi|} (\omega \otimes \rho)(X_{\pi(1)}, \dots, X_{\pi(k+\ell)}) \\ &= \sum_{\substack{\pi \in \mathbf{Perm}(k+\ell) \\ \pi(1) < \dots < \pi(k) \\ \pi(k+1) < \dots < \pi(k+\ell)}} (-1)^{|\pi|} \omega(X_{\pi(1)}, \dots, X_{\pi(k)}) \cdot \rho(X_{\pi(k+1)}, \dots, X_{\pi(k+\ell)}) \end{aligned} \tag{2.46}$$

$\forall X_i \in V$ . Given  $\omega, \rho \in \mathbf{Alt}^1V$ , for example,  $\omega \wedge \rho = \omega \otimes \rho - \rho \otimes \omega$ . With this definition, it is readily seen that the wedge product is associative, distributive, and anticommutative, such that

$$\omega \wedge \rho = (-1)^{k\ell} \rho \wedge \omega \tag{2.47}$$

for all  $\omega \in \mathbf{Alt}^kV$  and  $\rho \in \mathbf{Alt}^\ell V$ .

Defining the direct sum of alternating  $k$ -linear maps  $\mathbf{Alt}V = \bigoplus_k \mathbf{Alt}^kV$ , the wedge product defines  $\mathbf{Alt}V$  as an anticommuting graded algebra, called the *exterior algebra on  $V^*$* .

### 2.3.2 Differential forms

Moving now to the manifold picture, the exterior algebra  $\mathbf{Alt}T_mM$  may be defined in the usual manner by setting  $V = T_mM$  at each point  $m \in M$ , where  $\mathbf{dim}V = \mathbf{dim}M = n$ . The space  $\mathbf{Alt}^kT_mM \subset T_m^{(0,k)}M$  then consists of the totally antisymmetric  $(0, k)$  tensors at  $m$ . The subbundle  $\mathbf{Alt}^kTM \subset T^{(0,k)}M$  is now defined

by the collection of all such spaces,

$$\mathbf{Alt}^k TM = \bigcup_{m \in M} \mathbf{Alt}^k T_m M, \quad (2.48)$$

and it may also be viewed as a simple restriction of the  $(0, k)$  tensor bundle to its antisymmetric tensors.

Finally, *differential  $k$ -forms on  $M$*  (often simply,  *$k$ -forms*)—denoted  $\Lambda^k(M)$ —are defined to be the smooth sections of the alternating  $(0, k)$  tensor bundle, i.e.  $\Lambda^k(M) = \Gamma(\mathbf{Alt}^k TM)$ .  $k$ -forms inherit a pointwise exterior algebra from the spaces  $\mathbf{Alt}^k T_m M$ , so that wedge products are defined pointwise in the obvious way.  $k$  is also called the *degree* of a  $k$ -form.

Using their antisymmetry to advantage,  $k$ -forms can conveniently be expressed in local coordinates via the wedge product in a manner that makes their antisymmetry more explicit:

$$\omega = \omega_{a_1 \dots a_k} dx^{a_1} \otimes \dots \otimes dx^{a_k} = \frac{1}{k!} \omega_{a_1 \dots a_k} dx^{a_1} \wedge \dots \wedge dx^{a_k}. \quad (2.49)$$

When  $\omega$  is a top form (that is, a form of degree  $n = \mathbf{dim} M$ ), the antisymmetry of  $\omega$  lends itself to an additional simplification:

$$\omega = \frac{1}{n!} \omega_{a_1 \dots a_n} dx^{a_1} \wedge \dots \wedge dx^{a_n} = \omega_{1 \dots n} dx^1 \wedge \dots \wedge dx^n \quad (2.50)$$

so that no sum over indices need be implied.

There exists an  $\binom{n}{k}$ -dimensional basis induced by local coordinates for  $k$ -forms on a local coordinate chart  $(U, x)$ —that is, for  $\Lambda^k(U \subset M)$  regarded as a  $C^\infty(M)$  module—given by  $\left\{ dx^{\sigma(1)} \wedge \dots \wedge dx^{\sigma(k)} \mid \sigma \in \vec{\Sigma}_k^n \right\}$ .

Despite their technical definition presented here, differential forms turn out to be quite natural in that they are precisely those objects which can be integrated

over oriented manifolds. To see this, recall that an orientation-preserving change of coordinates  $x \rightarrow x(x')$  (where  $x$  is now viewed as a function of  $x'$ ) for the integral of a function  $f(x)$  is given by:

$$\int_M f(x) dx^1 \cdots dx^n = \int_{M'} f(x(x')) \mathbf{det} \left( \frac{\partial x}{\partial x'} \right) dx^{1'} \cdots dx^{n'} \quad (2.51)$$

where  $x(M') = M$  and  $\mathbf{det} \left( \frac{\partial x}{\partial x'} \right)$  denotes the Jacobian of the coordinate transformation. Serendipitously, as the result of its antisymmetry, an  $n$ -form transforms in the very same way. In particular, using the expression in Eq. (2.50):

$$\begin{aligned} \omega &= \omega_{1\dots n}(x) dx^1 \wedge \cdots \wedge dx^n \\ &= \omega_{1\dots n}(x(x')) \left( \frac{\partial x^1}{\partial x^{a'_1}} \cdots \frac{\partial x^n}{\partial x^{a'_n}} dx^{a'_1} \wedge \cdots \wedge dx^{a'_n} \right) \\ &= \omega_{1\dots n}(x(x')) \mathbf{det} \left( \frac{\partial x}{\partial x'} \right) dx^{1'} \wedge \cdots \wedge dx^{n'}. \end{aligned} \quad (2.52)$$

Here, the second line follows by the chain rule and by rewriting the function  $\omega_{1\dots n}(x)$  in terms of the new variable  $x'$ . The third line follows from the definition of the determinant. Since  $\omega$  can also be expressed in arbitrary coordinates— $\omega = \omega_{1'\dots n'}(x') dx^{1'} \wedge \cdots \wedge dx^{n'}$ —it follows that  $\omega_{1'\dots n'}(x') = \omega_{1\dots n}(x(x')) \mathbf{det} \left( \frac{\partial x}{\partial x'} \right)$  as necessary in Eq. (2.51).

Thus, integration may be geometrically *defined* on an oriented  $n$ -dimensional manifold specifically as an operation on differential  $n$ -forms. In particular, for an  $n$ -form defined in a local coordinate chart  $(U \subset M, x)$  on a manifold  $M$  such that  $\omega = \omega_{1\dots n}(x) dx^1 \wedge \cdots \wedge dx^n$ , its integral is defined by

$$\int_U \omega = \int_{V \subset \mathbb{R}^n} \omega_{1\dots n}(x) dx^1 \cdots dx^n, \quad (2.53)$$

where  $V = x(U) \subset \mathbb{R}^n$ . Since  $\omega$  transforms appropriately, this integral is independent of the coordinatization.

It is also worth noting that  $\Lambda^k(M)$  is clearly a  $C^\infty(M)$ -module, closed under addition and  $C^\infty(M)$ -multiplication. The 0-forms are simply smooth functions,  $\Lambda^0(M) = C^\infty(M)$ , while  $n$ -forms are volume forms (or ‘top forms’) on the  $n$ -dimensional manifold  $M$ . Lastly,  $\Lambda^{k>n}(M) = 0$  for  $\mathbf{dim}M = n$ , since indices will be forced to repeat in the antisymmetric components of the form.

### 2.3.3 Pullback

Just as vector fields were naturally ‘pushed forward’ by maps between manifolds, differential forms are naturally ‘pulled back.’

In particular, consider a differential  $k$ -form  $\beta \in \Lambda^k(N)$  and a smooth map  $f : M \rightarrow N$ . The *pullback* of  $\beta$  to  $M$ , denoted  $f^*\beta \in \Lambda^k(M)$ , is defined as the  $k$ -form on  $M$  such that

$$(f^*\beta)\Big|_m(X_1, \dots, X_k) = \beta\Big|_{f(m)}(f_*X_1, \dots, f_*X_k) \quad (2.54)$$

$\forall x \in M, X_i \in \mathfrak{X}(M)$ . For  $\beta \in \Lambda^0(M)$  a 0-form,  $f^*\beta = \beta \circ f$ . By its definition, the pullback  $f^* : \Lambda^k(N) \rightarrow \Lambda^k(M)$  is clearly a linear map. Note that the pullback is defined in terms of the pushforward; unlike the pushforward, however, the pullback  $f^*\omega$  of a  $k$ -form is a  $k$ -form for any smooth  $f$ . (Whereas the pushforward  $f_*X$  of a vector field  $X$  is only a vector field for  $f$  a diffeomorphism).

Integration behaves naturally under the pullback. In particular, using local coordinates it is straightforward to show that

$$\int_M f^*\omega = \int_N \omega \quad (2.55)$$

is just a geometric (coordinate-free) reexpression of the multiple integral change of variables formula, Eq. (2.51). The pullback also distributes over wedge products, such

that

$$f^*(\alpha \wedge \beta) = f^*\alpha \wedge f^*\beta \quad (2.56)$$

$$\forall \alpha \in \Lambda^k(M), \beta \in \Lambda^\ell(M).$$

### 2.3.4 Interior product

The *interior product* of a vector  $Y \in \mathfrak{X}(M)$  and a  $k$ -form  $\omega \in \Lambda^k(M)$ —denoted  $Y \lrcorner \omega$  or  $\iota_Y \omega$ —is defined as the  $(k - 1)$ -form satisfying

$$(Y \lrcorner \omega)(X_1, \dots, X_{k-1}) = \omega(Y, X_1, \dots, X_{k-1}). \quad (2.57)$$

The interior product is bilinear in both its arguments, and satisfies

$$\begin{aligned} Y \lrcorner (\omega \wedge \rho) &= (Y \lrcorner \omega) \wedge \rho + (-1)^k \omega \wedge (Y \lrcorner \rho) \quad \forall \omega \in \Lambda^k(M) \\ \iota_{[X,Y]} \Omega &= [\mathcal{L}_X, \iota_Y] \Omega. \end{aligned} \quad (2.58)$$

### 2.3.5 Exterior derivative

Given a  $k$ -form expressed in local coordinates,  $\omega = \omega_{1\dots k} dx^1 \wedge \dots \wedge dx^k$ , the *exterior derivative* of  $\omega$ —denoted  $d\omega$ —is a  $(k + 1)$ -form defined by

$$d\omega = \left( \frac{\partial}{\partial x^i} \omega_{1\dots k} \right) dx^i \wedge dx^1 \wedge \dots \wedge dx^k. \quad (2.59)$$

From the definition, it can be readily seen that  $d : \Lambda^k(M) \rightarrow \Lambda^{k+1}(M)$  is a linear anti-derivation that satisfies a closure property, i.e.

$$\begin{aligned}
d(a\omega + b\omega') &= ad\omega + bd\omega' \\
d(\omega \wedge \rho) &= d\omega \wedge \rho + (-1)^k \omega \wedge d\rho \\
d(d\omega) &= 0 \qquad \qquad \qquad \forall a, b \in \mathbb{R}, \omega, \omega' \in \Lambda^k(M), \rho \in \Lambda^\ell(M).
\end{aligned} \tag{2.60}$$

For  $f \in \Lambda^0(M)$ —that is,  $f \in C^\infty(M)$ —it is also apparent that  $df = f_*$ , since in local coordinates

$$\begin{aligned}
df(X) &= X_i \partial_i f \\
(f_*X)(h) = X(h \circ f) &= \left( X^i \partial_i f \frac{d}{ds} \right) h \quad \Rightarrow \quad (f_*X) = X^i \partial_i f \frac{d}{ds}.
\end{aligned} \tag{2.61}$$

(Although formally  $df(X) \in C^\infty(M)$  and  $f_*X \in \Gamma_{\text{loc}}(T\mathbb{R})$  live in different spaces, Eq. (2.61) implicitly identifies (i)  $\mathbb{R}$ , the target space of  $f$ , with (ii) the 1-dimensional vector space with basis  $\{\frac{d}{ds}\}$ , as local sections above a coordinate patch of  $M$ , as is natural.) The pushforward of a fixed vector field  $X \in \mathfrak{X}(M)$  along  $f : M \rightarrow N$  is also correspondingly expressed as

$$f_*X = df \circ X \circ f^{-1}, \tag{2.62}$$

where  $f^{-1}$  is appropriately restricted to an invertible subset of  $\mathbf{Im}f$ .

It can be shown that the exterior derivative—as defined by Eq. (2.59) in local coordinates—is the unique map  $\Lambda^k(M) \rightarrow \Lambda^{k+1}(M)$  that satisfies Eq. (2.60) and also  $df = f_*$  on  $f \in \Lambda^0(M)$ . Therefore, it must also have a coordinate-free expression,

which turns out to be

$$\begin{aligned}
(d\omega)(X_1, \dots, X_{k+1}) &= \sum_{i=1}^{k+1} (-1)^{k+1} X_i \left( \omega(X_1, \dots, \hat{X}_i, \dots, X_{k+1}) \right) \\
&\quad + \sum_{i < j} (-1)^{i+j} \omega \left( ([X_i, X_j], X_1, \dots, \hat{X}_i, \dots, \hat{X}_j, \dots, X_{k+1}) \right)
\end{aligned} \tag{2.63}$$

where  $\hat{X}_i$  denotes the omission of vector argument  $X_i$ . Here  $X_i \left( \omega(X_1, \dots, \hat{X}_i, \dots, X_{k+1}) \right)$  denotes a vector field differentiating a function, as in Eq. (2.31).

It is also worth noting that  $d$  behaves naturally with respect to pullbacks. In particular, given  $\omega \in \Lambda^k(N)$  and  $f : M \rightarrow N$ ,

$$d(f^*\omega) = f^*d\omega. \tag{2.64}$$

This is straightforwardly shown for  $\omega \in \Lambda^0(M)$ , since

$$d(f^*\omega) = d(\omega \circ f) = d\omega \circ df = d\omega \circ f_* = f^*d\omega. \tag{2.65}$$

(Here,  $d(\omega \circ f) = d\omega \circ df$  follows from Eq. (2.38).) Higher degree demonstrations of Eq. (2.64) then follow from the properties of Eq. (2.60).

A  $k$ -form  $\omega \in \Lambda^k(M)$  is said to be *closed* if

$$d\omega = 0. \tag{2.66}$$

$\omega \in \Lambda^k(M)$  is further said to be *exact* if

$$\omega = d\rho \tag{2.67}$$

for some  $\rho \in \Lambda^{k-1}(M)$ . Due to the last property of Eq. (2.60), all exact forms are clearly closed, however, closed forms need not be exact. A nice such counterexample arises on the punctured plane  $\mathbb{R}^2 \setminus \{0\}$  where the 1-form

$$d\theta = \frac{xdy - ydx}{x^2 + y^2} \quad (2.68)$$

is readily seen to be closed but not exact; after all, the polar coordinate  $\theta$  can either be regarded as multi-valued or discontinuous at  $\theta = 0, 2\pi, 4\pi, \dots$  but in any case  $\theta \notin C^\infty(M)$ .

### 2.3.6 Lie derivative

Another important derivation on a manifold  $M$  is now described. While an exterior derivative changes (by +1) the degree of a  $k$ -form, a Lie derivative, which is defined to act more generally on arbitrary  $(p, q)$  tensors, leaves tensorial degree unchanged.

It is often of interest to know how a tensor changes along the flow  $\exp(sX)$  induced by a vector field  $X$ . This is computed by the *Lie derivative with respect to  $X$* , denoted  $\mathcal{L}_X$ . For the simplest case of a function  $f \in C^\infty(M)$ , for example, one might wish to understand how  $f$  changes infinitesimally at a point  $m \in M$  along the flow of  $X$ , i.e.

$$\begin{aligned} \mathcal{L}_X(f) &= \left. \frac{d}{ds} \right|_{s=0} \left[ f(\exp(sX)m) \right] \\ &= \left. \frac{\partial f}{\partial x^i} \right|_m \left. \frac{d}{ds} \right|_{s=0} (\exp(sX)m)^i \stackrel{(2.35)}{=} \left. \frac{\partial f}{\partial x^i} \right|_m X_m^i = X(f) \Big|_m. \end{aligned} \quad (2.69)$$

For a function, therefore, the Lie derivative  $\mathcal{L}_X$  recovers the directional derivative as

described in Section 2.1.4.<sup>(\*)</sup>

To extend this notion to an arbitrary tensor field  $\sigma \in \Gamma(T^{(p,q)}M)$ , the Lie derivative of  $\sigma$  with respect to  $X \in \mathfrak{X}(M)$  is defined by

$$\mathcal{L}_X(\sigma) = \frac{d}{ds} \Big|_{s=0} \exp(sX)^* \sigma \quad (2.72)$$

such that, pointwise,  $\mathcal{L}_X(\sigma) \Big|_m = \lim_{s \rightarrow 0} \frac{\exp(sX)^*(\sigma|_{\exp(sX)m}) - \sigma|_m}{s}$ .

The pullback  $\exp(sX)^*$  ensures that  $\sigma$  is not compared in two distinct vector spaces but rather pulls the ‘upstream’ tensor in  $T_{\exp(sX)m}^{(p,q)}M$  back to  $T_m^{(p,q)}M$ . For  $\sigma \in \Gamma(T^{(0,1)}M)$ , this pullback is already defined by Eq. (2.54). For  $\sigma \in \mathfrak{X}(M)$ , the pullback is defined by inverting the pushforward, that is,  $\exp(sX)^*Y = \exp(-sX)_*Y$ . The pullback of a general  $\sigma \in \Gamma(T^{(p,q)}M)$  is then simply defined so that every upper index is pulled back as a vector field, and every lower index is pulled back as a covector field.

A number of useful properties of  $\mathcal{L}_X$  readily follow from its definition, including:

$$\begin{aligned} \mathcal{L}_X(\omega) &= d(X \lrcorner \omega) + X \lrcorner (d\omega) & \mathcal{L}_X(Y \lrcorner \omega) &= (\mathcal{L}_X Y) \lrcorner \omega + Y \lrcorner (\mathcal{L}_X \omega) \\ \mathcal{L}(\omega \wedge \rho) &= \mathcal{L}(\omega) \wedge \rho + \omega \wedge \mathcal{L}(\rho) & \mathcal{L}_X Y &= [X, Y]. \\ \mathcal{L}_X(d\omega) &= d(\mathcal{L}_X \omega) \end{aligned} \quad (2.73)$$

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<sup>(\*)</sup> As an aside, it bears noting that by Taylor’s theorem,

$$\begin{aligned} f(\exp(sX)m) &= f(m) + s \frac{d}{ds} \Big|_{s=0} [f(\exp(sX)m)] + \mathcal{O}(s^2) \\ &\stackrel{(2.69)}{=} f(m) + sX(f) \Big|_m + \mathcal{O}(s^2). \end{aligned} \quad (2.70)$$

Carrying this expansion to infinite order, it is found that

$$f(\exp(sX)m) = \sum_{k=0}^{\infty} \frac{s^k}{k!} X^k(f), \quad (2.71)$$

justifying the exponential notation for flows of Eq. (2.34).

### 2.3.7 de Rham Cohomology

A sequence of vector spaces and maps  $V_1 \xrightarrow{f_1} V_2 \xrightarrow{f_2} \dots \xrightarrow{f_{n-1}} V_n$  is said to be a *complex* if  $f_{i+1} \circ f_i = 0 \forall i$ , or equivalently, if  $\mathbf{Im} f_i \subseteq \mathbf{Ker} f_{i+1} \forall i$  (where  $\mathbf{Im}$  and  $\mathbf{Ker}$  denote image and kernel, respectively). A complex is moreover said to be *exact* if  $\mathbf{Im} f_i = \mathbf{Ker} f_{i+1} \forall i$ .

The closure property  $d \circ d = 0$  of the exterior derivative, as noted in Eq. (2.60), affords the existence of the *de Rham complex* of differential forms on an  $n$ -dimensional manifold  $M$ , defined as

$$0 \hookrightarrow \mathbb{R} \hookrightarrow \Lambda^0(M) \xrightarrow{d} \Lambda^1(M) \xrightarrow{d} \dots \xrightarrow{d} \Lambda^n(M) \xrightarrow{d} 0. \quad (2.74)$$

Here,  $\mathbb{R} \hookrightarrow \Lambda^0(M)$  denotes the inclusion map to constant functions on  $M$ . It is useful to label the exterior derivatives between spaces such that  $d_k$  denotes the map  $\Lambda^k(M) \xrightarrow{d_k} \Lambda^{k+1}(M)$ .

The sets of closed and exact  $k$ -forms, respectively, are typically denoted<sup>(\*)</sup>

$$\begin{aligned} Z^k(M) &= \mathbf{Ker} d_k = \left\{ \omega \in \Lambda^k(M) \mid d_k \omega = 0 \right\} \\ B^k(M) &= \mathbf{Im} d_{k-1} = \left\{ \omega \in \Lambda^k(M) \mid \exists \rho, \omega = d_{k-1} \rho \right\} = d_{k-1} \Lambda^{k-1}(M). \end{aligned} \quad (2.75)$$

Clearly,  $B^k(M) \subseteq Z^k(M)$ .

The  $k^{\text{th}}$  *cohomology group* of  $M$ , denoted  $H^k(M)$ , is defined as the set of closed forms modulo the exact forms, that is:

$$H^k(M) = \frac{Z^k(M)}{B^k(M)}. \quad (2.76)$$

An element  $[\omega] = \omega + d_{k-1} \Lambda^{k-1} \in H^k(M)$  denotes an equivalence class of  $k$ -forms whose exact term can be arbitrary. The de Rham complex is exact precisely when

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<sup>(\*)</sup>  $Z$  is derived from the German “zyklus” for “cycle” while  $B$  suggests “boundary.”

$H^k(M) = 0 \forall k$ , and its non-exactness remarkably conveys purely topological information about the manifold  $M$ . In fact, it should be noted that a closed form is always locally exact in a small enough, (topologically uninteresting) neighborhood. However, there is no guarantee that a closed form is globally exact—as seen in Eq. (2.68).

A result closely connected to the de Rham complex is a powerful theorem in integration known as *Stokes' theorem*,<sup>(\*\*)</sup> which holds that for a compact, oriented  $n$ -dimensional manifold  $M$  with boundary  $\partial M$ ,

$$\int_M d\omega = \int_{\partial M} \omega \tag{2.77}$$

$\forall \omega \in \Lambda^{n-1}(M)$ .

## 2.4 (Pseudo)-Riemannian manifolds

### 2.4.1 Metric

A great deal of geometrical structure follows from the introduction of a metric  $g$  on a smooth manifold  $M$ , an object that shall be collectively denoted  $(M, g)$ . A *pseudo-Riemannian metric* is defined as any nondegenerate symmetric  $(0, 2)$ -tensor field  $g \in \Gamma(T^{(0,2)}M)$ , such that  $\forall m \in M, g(X, Y)|_m = 0 \forall Y \in \mathfrak{X}(M)$  implies  $X = 0$ . A manifold  $M$  equipped with such a metric is further said to be a *pseudo-Riemannian manifold*. If  $g$  is also positive definite—i.e.  $g(X, X)|_m > 0 \forall m \in M, (X \neq 0) \in \mathfrak{X}(M)$ —then  $(M, g)$  is called a *Riemannian manifold*. Hereafter,  $(M, g)$  will be assumed pseudo-Riemannian.

The metric  $g$  endows each tangent space  $T_m M$  with a nondegenerate, symmetric 2-form, namely  $g(X, Y)|_m$ . This 2-form effectuates a notion of distance on  $M$ ,

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<sup>(\*\*)</sup> Stokes' theorem demonstrates that the cohomology of the de Rham complex (defined via  $d$ ) is dual to the homology of the chain complex (defined via the boundary operator,  $\partial$ ) on a manifold  $M$ , with the pairing between these dual spaces defined by integration.

wherein an infinitesimal *line element*  $d\ell$  in the direction of  $X_m$  is conceived to have ‘squared infinitesimal distance’  $d\ell^2 = g(X_m, X_m)$ . Summing (the square root of) such infinitesimal contributions along an integral curve of  $X$  on  $M$  measures its distance. In local coordinates (denoted by convention with Greek indices on pseudo-Riemannian manifolds) for example, letting  $X = \frac{dx^\mu}{ds} \frac{\partial}{\partial x^\mu}$

$$\Delta\ell = \int d\ell = \int ds \sqrt{g_{\mu\nu} \frac{dx^\mu}{ds} \frac{dx^\nu}{ds}}. \quad (2.78)$$

A metric also endows each tangent space  $T_m M$  with a notion of orthonormality. Specifically, a basis  $\{e_1, \dots, e_n\}$  of  $T_m M$  is said to be *orthonormal with respect to  $g$*  if  $g(e_\mu, e_\nu)|_m = \pm\delta_{\mu\nu}$ . Since  $g$  is symmetric (and thus diagonalizable) and nondegenerate, such a basis can always be found.

The *signature*  $\mathbf{Sig}(g) = (p, q)$  of  $g$  is defined by the number  $p$  (or  $q$ ) of ‘positive’ (or ‘negative’) orthonormal basis vectors  $\{e_\mu\}$  such that  $g|_m(e_\mu, e_\mu) = 1$  (or  $-1$ ). The *index*  $\mathbf{Ind}(g)$  of  $g$  denotes the number of ‘negative’ such basis vectors. By the smoothness and nondegeneracy of  $g$ , these are constant from point to point.

The paradigmatic example of a pseudo-Riemannian metric is defined by *Minkowski spacetime*  $(\mathbb{R}^{3,1}, \eta)$ . In  $(t, x, y, z)$  coordinates, its metric is given by

$$\eta_{\mu\nu} = \begin{pmatrix} -1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{pmatrix} \quad (2.79)$$

such that  $\mathbf{Sig}(\eta) = (3, 1)$  and  $\mathbf{Ind}(\eta) = 1$ .

## 2.4.2 Hodge star

While differential forms are topological objects that can exist independent of a metric, their interaction with a metric is often mediated via the Hodge star, denoted  $\star$ . This is a metric-induced map between  $k$ -forms and  $(n - k)$ -forms.

To define  $\star$ , first note that an oriented,  $n$ -dimensional manifold  $(M, g)$  has a unique  $n$ -form (a *volume form* or *top form*) denoted  $\mathbf{vol}_g \in \Lambda^n(M)$  such that  $\mathbf{vol}_g(e_1, \dots, e_n) = 1$  for any positively oriented orthonormal basis  $\{e_\mu\}$ . (Recall that  $\Lambda^n(M)$  is 1-dimensional so that this uniqueness is a matter of simply choosing  $f(x) = 1$  in  $\mathbf{vol}_g = f(x)dx^1 \wedge \dots \wedge dx^n$ .)

Furthermore, note that the metric on  $(M, g)$  also pointwise induces a symmetric nondegenerate form  $(\cdot, \cdot)_{\Lambda^k}$  on  $\Lambda^k(M) \forall k \in \{1, \dots, n\}$  in the following way. In local coordinates, for  $\omega, \rho \in \Lambda^k(M)$ ,

$$\begin{aligned} (\omega, \rho)_{\Lambda^k} &= \frac{1}{k!} \omega_{\mu_1 \dots \mu_k} \rho^{\mu_1 \dots \mu_k} \\ &= \frac{1}{k!} \omega_{\mu_1 \dots \mu_k} \rho_{\nu_1 \dots \nu_k} g^{\mu_1 \nu_1} \dots g^{\mu_k \nu_k}. \end{aligned} \tag{2.80}$$

This form is symmetric and basis-independent.

The *Hodge star*  $\star : \Lambda^k(M) \rightarrow \Lambda^{n-k}(M)$  is then defined as the unique isomorphism satisfying

$$(\omega, \rho)_{\Lambda^k} \mathbf{vol}_g = \omega \wedge \star \rho \tag{2.81}$$

$\forall \omega, \rho \in \Lambda^k(M)$ . Since  $(\omega, \rho)_{\Lambda^k}$  is symmetric, it follows that  $\omega \wedge \star \rho = \rho \wedge \star \omega$ . Furthermore, it is readily calculated that

$$\star \star \omega = (-1)^{\mathbf{Ind}(g)} (-1)^{k(n-k)} \omega, \tag{2.82}$$

verifying that  $\star$  is an isomorphism.

### 2.4.3 Codifferential

The symmetric form  $(\cdot, \cdot)_{\Lambda^k}$  on  $k$ -forms defined pointwise  $\forall m \in M$  can be naturally extended to a symmetric form  $(\cdot, \cdot)_{L^2\Lambda^k}$  on  $k$ -forms over all of  $M$ . In particular, define

$$(\omega, \rho)_{L^2\Lambda^k} = \int_M (\omega, \rho)_{\Lambda^k} \mathbf{vol}_g = \int_M \omega \wedge \star \rho. \quad (2.83)$$

Further define the *codifferential*  $\delta : \Lambda^k(M) \rightarrow \Lambda^{k-1}(M)$  as the map satisfying

$$\star \delta \omega = (-1)^k d \star \omega \quad (2.84)$$

$\forall \omega \in \Lambda^k(M)$ .

Then, note that Stokes' theorem of Eq. (2.77) combined with the Leibniz rule for the exterior derivative of Eq. (2.60) implies

$$\begin{aligned} \int_{\partial M} \omega \wedge \star \rho &= \int_M d(\omega \wedge \star \rho) = \int_M [d\omega \wedge \star \rho + (-1)^k \omega \wedge d \star \rho] \\ &= (d\omega, \rho)_{L^2\Lambda^k} - (\omega, \delta \rho)_{L^2\Lambda^k} \end{aligned} \quad (2.85)$$

$\forall \omega \in \Lambda^k(M), \rho \in \Lambda^{k+1}(M)$ . Up to a boundary term, therefore,  $\delta$  is a formal adjoint of the exterior derivative  $d$  under  $(\cdot, \cdot)_{L^2\Lambda^k}$ . After all, modulo the boundary term of Eq. (2.85)

$$(d\omega, \rho)_{L^2\Lambda^k} = (\omega, \delta \rho)_{L^2\Lambda^k}. \quad (2.86)$$

## 2.5 Lie groups, Lie algebras, group actions and representations

### 2.5.1 Lie groups

A critical role is played in physics by Lie groups, mathematical objects that are simultaneously geometric smooth manifolds and algebraic groups. A *group* is a set  $G$  equipped with a binary operation  $(\cdot)$  satisfying four axioms:

- (a) *Closure.* For any  $g, h \in G$ ,  $g \cdot h \in G$ .
- (b) *Identity.* There exists a distinguished element  $\mathbb{1}$  of  $G$  (the *identity*) satisfying
$$\mathbb{1} \cdot g = g \cdot \mathbb{1} = g.$$
- (c) *Inverse.* For any  $g \in G$  there exists  $g^{-1} \in G$  (the *inverse of g*) satisfying
$$g^{-1} \cdot g = g \cdot g^{-1} = \mathbb{1}.$$
- (d) *Associativity.* For any  $g, h, k \in G$ ,  $g \cdot (h \cdot k) = (g \cdot h) \cdot k$ .

Hereafter, the identity of a group will sometimes be denoted  $e$  instead of  $\mathbb{1}$ . A product of elements of  $G$  will also simply be written  $gh$  at times. A group is said to be *abelian* if  $gh = hg \forall g, h \in G$ , (and *nonabelian* otherwise).

Groups often arise naturally as a set of symmetry transformations. The dihedral group  $D_3$ , for example, is the set of six symmetry transformations of an equilateral triangle, defined by three rotations (in multiples of  $120^\circ$ ) and three reflections through its perpendicular bisectors. It is readily checked that these six transformations satisfy the group axioms.

As a second example, the two-dimensional Euclidean plane is invariant under rotations and translations. These symmetries indeed *define* the Euclidean plane.<sup>(\*)</sup>

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<sup>(\*)</sup> For example, contrast the Euclidean plane with the Cartesian plane defined with points labeled by  $(x, y)$  coordinates. The Cartesian plane has no symmetries, since no (nontrivial) transformation of the plane leaves this labeling invariant. The Euclidean plane is abstracted away from coordinatization, and its resulting symmetries render it a foundational geometric object.

The set of all compositions of rotations and translations is called the *special Euclidean group*, denoted  $SE(2)$ . (The  $S$  indicates that reflections of the plane are omitted, such that  $SE(2)$  is orientation-preserving.)

A Lie group is a specialization of groups to those that have a smooth manifold structure. In particular, an *n-dimensional Lie group* is a group  $G$  that is also an  $n$ -dimensional smooth manifold, such that the functions  $\mu$  and  $\iota$  denoting group composition—

$$\begin{aligned} \mu : G \times G &\rightarrow G \\ (g, h) &\mapsto \mu(g, h) = g \cdot h \quad \forall g, h \in G \end{aligned} \tag{2.87}$$

—and inversion—

$$\begin{aligned} \iota : G &\rightarrow G \\ g &\mapsto \iota(g) = g^{-1} \quad \forall g \in G \end{aligned} \tag{2.88}$$

—are smooth maps between manifolds.

An important example of a Lie group is the *general linear group*  $GL(V)$ , consisting of all automorphisms of a vector space  $V$  under composition:  $g_1 \bullet g_2 = g_1 \circ g_2$ . When  $V = \mathbb{R}^n$  for  $n < \infty$ ,  $GL(V)$  is denoted  $GL(n, \mathbb{R})$  or  $GL_n(\mathbb{R})$ , the group of  $n \times n$  invertible real matrices. (A corresponding treatment follows for  $V = \mathbb{C}^n$ .) Composition is given by matrix multiplication.

A *Lie group homomorphism*  $\phi : G \rightarrow H$  is a smooth map between Lie groups satisfying  $\phi(gh) = \phi(g)\phi(h)$ . If  $\phi$  is also bijective, it is called a *Lie group isomorphism*. A *subgroup* of a Lie group  $G$  is any Lie group  $H \subset G$  whose group composition law is inherited from  $G$ .

Many more Lie groups arise as closed subgroups of  $GL(n, \mathbb{R})$  or  $GL(n, \mathbb{C})$ . These are called *matrix Lie groups*, for example:

- (a)  $SL(n, \mathbb{R}) = \left\{ A \in GL(n, \mathbb{R}) \mid \mathbf{det} A = 1 \right\}$  denotes the real special linear group.
- (b)  $SL(n, \mathbb{C}) = \left\{ A \in GL(n, \mathbb{C}) \mid \mathbf{det} A = 1 \right\}$  denotes the complex special linear group.
- (c)  $O(p, q) = \left\{ O \in GL(p+q, \mathbb{R}) \mid O^T \eta_{p,q} O = \eta_{p,q} \right\}$  denotes the (*indefinite*) *orthogonal group* preserving a bilinear form of signature  $(p, q)$ , namely

$$\eta_{p,q} = \begin{bmatrix} \mathbb{1}_p & \\ & -\mathbb{1}_q \end{bmatrix}, \quad (2.89)$$

where  $\mathbb{1}_p$  denotes the  $p \times p$  identity matrix. In particular, for vectors  $v, w \in \mathbb{R}^{p+q}$ , it follows that

$$(v, w)_{p,q} = v^T \eta_{p,q} w = v^T O^T \eta_{p,q} O w = (Ov, Ow)_{p,q}. \quad (2.90)$$

- (d)  $SO(p, q) = \left\{ O \in O(p, q) \mid \mathbf{det} O = 1 \right\}$  denotes the *special orthogonal group* restricting  $O(p, q)$  to its orientation-preserving transformations.
- (e)  $U(p, q) = \left\{ U \in GL(p+q, \mathbb{C}) \mid U^\dagger \eta_{p,q} U = \eta_{p,q} \right\}$  denotes the (*indefinite*) *unitary group*, where  $U^\dagger = (U^*)^T$  denotes the conjugate transpose of  $U$ . Like its real counterpart  $O(p, q)$ , the group  $U(p, q)$  preserves an inner product given by  $\langle v, w \rangle_{p,q} = v^\dagger \eta_{p,q} w$ .
- (f)  $SU(p, q) = \left\{ U \in U(p, q) \mid \mathbf{det} U = 1 \right\}$  denotes the *special unitary group*.
- (g)  $Sp(2n, \mathbb{R}) = \left\{ A \in GL(2n, \mathbb{R}) \mid A^T \Omega A = \Omega \right\}$  denotes the *symplectic group* in  $2n$  dimensions, where

$$\Omega = \begin{bmatrix} & \mathbb{1}_n \\ -\mathbb{1}_n & \end{bmatrix}. \quad (2.91)$$

(h)  $Sp^*(2n, \mathbb{C}) = \left\{ A \in GL(2n, \mathbb{C}) \mid A^\dagger \Omega A = \Omega \right\}$  denotes the *conjugate symplectic group* in  $2n$  complex dimensions.

All of the above are clearly seen to be closed under matrix multiplication, and they are closed as sets in  $GL(d, \mathbb{R})$  or  $GL(d, \mathbb{C})$  for some  $d$  because they are each defined by a quadratic equation (e.g. the preservation of some bilinear form). The notation  $O(n) = O(n, 0)$  is used for the orthogonal group of strictly positive signature, (and likewise for all the other matrix groups).

## 2.5.2 Lie algebras

The manifold structure of a Lie group  $G$  begins to prove quite useful when its differential structure is investigated via its vector fields.

Vector fields that reflect the group structure of  $G$  can be constructed as follows. Given a Lie group  $G$ , one may define a *left translation* map  $\ell_g : G \rightarrow G$  such that  $\ell_g(h) = gh$ . Clearly  $\ell_g \circ \ell_h = \ell_{gh}$ . Although it is not a group isomorphism,  $\ell_g$  is a diffeomorphism (invertible and smooth). Thus, using the manifold structure of  $G$ , a vector field  $X \in \mathfrak{X}(G)$  can be pushed forward to  $\ell_{g*}X \in \mathfrak{X}(G)$ , such that  $(\ell_{g*}X)_{gh} = \ell_{g*}(X_h) \forall g, h \in G$ .

A vector field  $X \in \mathfrak{X}(G)$  is called *left-invariant* if  $\ell_{g*}X = X \forall g \in G$ , that is, if  $X$  is preserved by left translation. Pointwise, this can be written  $\ell_{g*}(X_h) = X_{gh}$ , or equivalently, as acting on a function  $f : G \rightarrow \mathbb{R}$  such that,  $\forall g, h \in G$

$$[X(f \circ \ell_g)](h) = X_h(f \circ \ell_g) = \left[ (\ell_{g*}X_h)f = X_{gh}f \right] = (Xf)(gh) = [(Xf) \circ \ell_g](h). \quad (2.92)$$

Therefore, the left-invariance of  $X$  is equivalent to demanding that

$$X(f \circ \ell_g) = (Xf) \circ \ell_g \quad (2.93)$$

$\forall g \in G, f \in C^\infty(G)$ . The set of left-invariant vector fields on  $G$  is denoted  $L(G) \subset \mathfrak{X}(G)$ . It is clear from the definition of Eq. (2.93) that  $L(G)$  is closed under addition and multiplication by  $\mathbb{R}$ , and is therefore a vector space.

It is moreover straightforward to see that left-invariance is preserved by the Jacobi-Lie bracket of Section 2.2.7, since, given  $X, Y \in \mathfrak{X}(G)$  left-invariant and repeatedly applying Eq. (2.93),

$$[X, Y](f \circ \ell_g) = X(Y(f \circ \ell_g)) - Y(X(f \circ \ell_g)) = [X, Y](f) \circ \ell_g \quad (2.94)$$

Therefore, as defined in Section 2.2.7,  $L(G)$  is a Lie algebra with a bracket imported from the Jacobi-Lie bracket on vector fields.

It turns out that  $L(G)$  can be cleanly characterized by noting that  $L(G) \cong T_e G$  are isomorphic as vector spaces, where  $T_e G$  denotes the tangent space over the identity. An isomorphism is explicitly given by

$$\begin{aligned} \phi : T_e G &\rightarrow L(G) \\ A &\mapsto \phi(A) = L^A \quad \text{where} \quad L_g^A = \ell_{g*} A. \end{aligned} \quad (2.95)$$

That is, a vector  $A \in T_e G$  can be uniquely pushed forward to a vector field  $L^A$  on  $G$  defined pointwise via left translation.  $L^A$  is left invariant since  $\ell_{g*} L_h^A = \ell_{g*} \ell_{h*} A = \ell_{gh*} A = L_{gh}^A$ . It is clear that  $\phi$  is surjective, since any left invariant vector field  $X$  satisfies  $X = \phi(X_e)$ , and  $\phi$  is injective because  $L^A = L^B$  implies  $A = L_e^A = L_e^B = B$ .

Therefore, the Lie algebra  $L(G)$  may be understood as the tangent space  $T_e G$  (also denoted  $\mathfrak{g}$ ) and equipped with a Lie bracket  $[[\cdot, \cdot]]$  induced by the Jacobi-Lie bracket of left-invariant vector fields. That is,

$$[[A, B]] = \phi^{-1}\left([\phi(A), \phi(B)]\right) \quad (2.96)$$

$\forall A, B \in T_e G$ . Note, this construction immediately implies that  $\mathbf{dim}L(G) = \mathbf{dim}T_e G = \mathbf{dim}G$ .

For a matrix Lie group  $G \subset GL(d, \mathbb{R})$ , for example, a local coordinate chart  $x : GL(d, \mathbb{R}) \rightarrow \mathbb{R}^{d \times d}$  can be chosen near  $e$  such that

$$x^i_j(g) = g^i_j \quad (2.97)$$

for  $i, j \in \{1, \dots, d\}$ . (Note that  $x(G)$  may occupy only a submanifold of  $x(GL(d, \mathbb{R}))$ , but that will not matter here.) Lie algebra matrix elements are then similarly specified as  $A = A^i_j \frac{\partial}{\partial x^i_j}$ . For a matrix Lie group,  $\ell_g$  acts linearly on its argument, so that  $\ell_{g_*} A = gA$ . Expressed in the chart  $x$ , therefore,  $\phi(A) = x^i_j A^j_k \frac{\partial}{\partial x^i_k}$  and  $[\phi(A), \phi(B)] = x^i_j (A^j_k B^k_\ell - B^j_k A^k_\ell) \frac{\partial}{\partial x^i_\ell}$  such that, applying  $\phi^{-1}$  (via left multiplication of  $g^{-1}$ ), the Lie bracket on  $\mathfrak{g}$  is given by

$$[[A, B]] = AB - BA, \quad (2.98)$$

$\forall A, B \in \mathfrak{g}$ . (Here, the notation  $[[\cdot, \cdot]]$  is used merely to distinguish the Lie bracket on  $\mathfrak{g}$  from the Jacobi-Lie bracket on vector fields.) The Lie bracket on a matrix Lie algebra is thus defined by the matrix commutator.

A *Lie algebra homomorphism* is defined as a linear map  $\phi : \mathfrak{g} \rightarrow \mathfrak{h}$  that preserves Lie brackets, i.e.

$$\phi([[A, B]]_{\mathfrak{g}}) = [[\phi(A), \phi(B)]]_{\mathfrak{h}}. \quad (2.99)$$

The *exponential map* on a Lie group  $G$  is defined by

$$\begin{aligned} \exp : \mathfrak{g} &\rightarrow G \\ A &\mapsto \exp(A)e \end{aligned} \quad (2.100)$$

where  $\exp(sA)e \forall s \in \mathbb{R}$  has a definition identical to the flow along a vector field, as defined in Eq. (2.34). For a matrix Lie algebra, the exponential map may be calculated as in Eq. (2.71) to be

$$\exp(sA) = \sum_{k=1}^{\infty} \frac{s^k}{k!} A^k. \quad (2.101)$$

Using the exponential map, it is straightforward to calculate the defining relationship of a Lie algebra corresponding to a matrix Lie group. In particular, it suffices to differentiate the defining relationship of the Lie group. For example, the Lie algebra  $\mathfrak{o}(p, q)$  of the matrix Lie group  $O(p, q)$  can be found via

$$\left. \frac{d}{ds} \right|_{s=0} \left[ \exp(sA)^T \eta_{p,q} \exp(sA) = \eta_{p,q} \right] \Rightarrow A^T \eta_{p,q} + \eta_{p,q} A = 0. \quad (2.102)$$

Expressions for other matrix Lie algebras follow similarly.

### 2.5.3 Lie group representations

A *representation*  $\rho : G \rightarrow GL(V)$  of a Lie group  $G$  is defined as a group homomorphism from  $G$  to  $GL(V)$ , the general linear group on a vector space  $V$ , called the *representation space* of  $\rho$  (or sometimes, simply, the *representation*).

An invariant subspace of a Lie group representation  $V$  is a subspace  $W \subset V$  such that  $\rho(G) \cdot W \subset W$ . A nonzero representation  $\rho$  is said to be *irreducible* if the only invariant subspaces are  $V$  and  $\{0\}$ .

The simplest representation of a matrix Lie group  $G \subset GL(d, \mathbb{R})$  is called the *fundamental representation*. It is given by the defining matrices of the group, acting on the representation space  $\mathbb{R}^d$ . For example, the fundamental representation of  $SO(3)$  is given by  $\rho : SO(3) \rightarrow GL(\mathbb{R}^3)$  where  $g \in SO(3)$  is mapped to itself, reinterpreted as a transformation on  $\mathbb{R}^3$ .

Every Lie group has a representation whose representation space is given by its

Lie algebra. Its construction proceeds as follows. Define the conjugation map

$$\begin{aligned} \mathbf{K}_g : G &\rightarrow G \\ h &\mapsto ghg^{-1}. \end{aligned} \tag{2.103}$$

Notably, since  $geg^{-1} = e$ ,  $\mathbf{K}_g$  fixes the identity element  $\forall g \in G$ . The pushforward of the conjugation map—denoted  $\mathbf{Ad}_g = \mathbf{K}_{g*}$ —therefore acts as an endomorphism on  $T_eG$ . To calculate its mapping of an element  $A \in T_eG$ , note that  $\forall f \in C^\infty(G)$ ,

$$\begin{aligned} [\mathbf{Ad}_g A] f(e) &= A(f \circ \mathbf{K}_g)(e) \\ &= \left. \frac{d}{ds} \right|_{s=0} (f \circ \mathbf{K}_g)(\exp(sA)e) \\ &= \left. \frac{d}{ds} \right|_{s=0} f(g \exp(sA)g^{-1}). \end{aligned} \tag{2.104}$$

where the second line simply applies the definition of a Lie derivative.

For a matrix Lie group  $G \subset GL(d, \mathbb{R})$ , Eq. (2.104) can be expressed in local coordinates as in Eq. (2.97), such that via the chain rule,

$$[\mathbf{Ad}_g A] f(e) = \left. \frac{\partial f}{\partial(x^i_\ell)} \right|_e \cdot (g^i_j A^j_k (g^{-1})^k_\ell) = (gAg^{-1})^i_j \left. \frac{\partial f}{\partial(x^i_j)} \right|_e \quad \Rightarrow \quad \mathbf{Ad}_g A = gAg^{-1}. \tag{2.105}$$

where  $g$ ,  $A$  and  $g^{-1}$  are multiplied as matrices. By construction, it is assured that  $gAg^{-1} \in T_eG$ .

Since the pushforward is covariant, as expressed in Eq. (2.38), and since  $\mathbf{K}_g \circ \mathbf{K}_h = \mathbf{K}_{gh}$ , the map

$$\begin{aligned} \mathbf{Ad} : G &\rightarrow GL(\mathfrak{g}) \\ g &\mapsto \mathbf{Ad}_g \quad \text{s.t.} \quad \mathbf{Ad}_g A = gAg^{-1} \end{aligned} \tag{2.106}$$

defines a group homomorphism, called the *adjoint representation of (a matrix group)*

$G$  with representation space  $\mathfrak{g}$ . Clearly,  $\text{Ad}_g$  is invertible with inverse  $\text{Ad}_{g^{-1}}$ .

Lastly, since  $G$  has a natural adjoint representation on  $\mathfrak{g}$ , and since  $\mathfrak{g}$  has a vector space dual  $\mathfrak{g}^*$ , a representation of  $G$  on  $\mathfrak{g}^*$  is induced. In particular, one may define a transformation dual to  $\text{Ad}_g$ , denoted  $\text{Ad}_g^* : \mathfrak{g}^* \rightarrow \mathfrak{g}^*$  and defined such that

$$\langle \text{Ad}_g^* \alpha, A \rangle = \langle \alpha, \text{Ad}_g A \rangle. \quad (2.107)$$

$\forall \alpha \in \mathfrak{g}^*$  and  $A \in \mathfrak{g}$ , where  $\langle \cdot, \cdot \rangle$  denotes the bilinear pairing of  $\mathfrak{g}^*$  and  $\mathfrak{g}$ .

To define a *left* group action using this dual map, one may define the *coadjoint action* of  $G$  on  $\mathfrak{g}^*$  such that

$$\begin{aligned} \Phi : G \times \mathfrak{g}^* &\rightarrow \mathfrak{g}^* \\ (g, \alpha) &\mapsto \text{Ad}_{g^{-1}}^* \alpha. \end{aligned} \quad (2.108)$$

(This defines a left group action because  $\langle \text{Ad}_{g^{-1}}^* \text{Ad}_h^* \alpha, A \rangle = \langle \alpha, \text{Ad}_{(gh)^{-1}} A \rangle = \langle \text{Ad}_{(gh)^{-1}}^* \alpha, A \rangle$ .)

Accordingly, this group action defines the *coadjoint representation* of  $G$  on  $\mathfrak{g}^*$ .

## 2.5.4 Lie algebra representations

Analogously, a *Lie algebra representation*  $\rho : \mathfrak{g} \rightarrow \mathbf{End}(V)$  is a Lie algebra homomorphism from a Lie algebra  $\mathfrak{g}$  to the (not necessarily invertible) endomorphisms on a vector space  $V$ , where the Lie bracket on  $\mathbf{End}(V)$  is defined by composition, i.e.

$$\rho\left([A, B]_{\mathfrak{g}}\right) = \rho(A) \circ \rho(B) - \rho(B) \circ \rho(A). \quad (2.109)$$

The adjoint representation of a Lie algebra  $\mathfrak{g}$  on itself can be derived by differentiating the adjoint representation  $\text{Ad}_g$  ‘with respect to  $g$ ,’ such that its differential at  $g = e$  comprises a representation of the Lie algebra. Restricting attention again to

matrix groups, given  $A, B \in \mathfrak{g}$ , the *adjoint representation* is derived by noting

$$\begin{aligned} \mathbf{ad}_A B &= \left. \frac{d}{ds} \right|_{s=0} \mathbf{Ad}_{\exp(sA)} B \\ &= \left. \frac{d}{ds} \right|_{s=0} \exp(sA) B \exp(-sA) = AB - BA. \end{aligned} \tag{2.110}$$

Therefore, the adjoint representation is given by

$$\begin{aligned} \mathbf{ad} : \mathfrak{g} &\rightarrow \mathbf{End}(\mathfrak{g}) \\ A &\mapsto \mathbf{ad}_A \quad \text{s.t.} \quad \mathbf{ad}_A B = [A, B]. \end{aligned} \tag{2.111}$$

That this is a Lie algebra homomorphism follows from the Jacobi identity, since

$$\mathbf{ad}_{[A,B]} C = [[A, B], C] = [A, [B, C]] - [B, [A, C]] = (\mathbf{ad}_A \circ \mathbf{ad}_B - \mathbf{ad}_B \circ \mathbf{ad}_A) C. \tag{2.112}$$

The fundamental representation of a matrix Lie algebra  $\mathfrak{g} \subset \mathfrak{gl}(d, \mathbb{R})$ , much like its Lie group counterpart, is simply defined by reinterpreting its own elements as transformations on a vector space  $\mathbb{R}^d$ .

### 2.5.5 Group actions on manifolds

While the last few sections briefly described group transformations in their natural setting of representations, a considerably more general class of group transformations is defined via group actions on manifolds.

Given a Lie group  $G$  and a manifold  $M$ , a *group action* of  $G$  on  $M$  is defined as a smooth map

$$\begin{aligned} \Phi : G \times M &\rightarrow M \\ (g, m) &\mapsto \Phi(g, m) = g \cdot m \end{aligned} \tag{2.113}$$

satisfying

$$(a) \quad \Phi(g, \Phi(h, m)) = \Phi(gh, m) \quad \forall g, h \in G, m \in M$$

$$(b) \quad \Phi(\mathbb{1}, m) = m \quad \forall m \in M.$$

For a fixed element  $g \in G$ , its group action on  $M$  is denoted  $\Phi_g : M \rightarrow M$  such that  $\Phi_g(m) = \Phi(g, m)$ . From condition (a), it follows that  $\Phi_g \circ \Phi_h = \Phi_{gh}$ . Such a group action is therefore called a *left action*, and denoted  $\Phi_g(m) = g \cdot m$  or  $\Phi_g(m) = g \triangleright m$ . A *right action*, by contrast, modifies the right hand side (RHS) of condition (a) above to  $\Phi(g, \Phi(h, m)) = \Phi(hg, m)$  so that it satisfies  $\Phi_g \circ \Phi_h = \Phi_{hg}$ . A right action can be denoted  $\Phi_g(m) = m \cdot g$  or  $\Phi_g(m) = m \triangleleft g$ .

Referring back to the definition of flow for a vector field, Eq. (2.35) demonstrates that the vector field flow  $\{\exp(sX) : M \rightarrow M\}$  constitutes a group action on the manifold  $M$ , where  $\exp(sX)$  is regarded as an element of a one-dimensional abelian Lie group under composition.

Furthermore, in Eq. (2.35) the tangent vector to the flow was identified as the generator of the group action of  $\exp$ , since  $\forall m \in M, X_m = \left. \frac{d}{ds} \right|_{s=0} \exp(sX)m$ . Generalizing to the arbitrary group action  $\Phi$  of a Lie group  $G$  as in Eq. (2.113), the *infinitesimal generator* of the group action  $\Phi$  corresponding to a Lie algebra element  $A \in \mathfrak{g}$  is defined pointwise on  $M$  by

$$X_m^A = \left. \frac{d}{ds} \right|_{s=0} \Phi_{\exp(sA)}(m). \quad (2.114)$$

In this way, a group action associates to each  $A \in \mathfrak{g}$  a vector field  $X^A \in \mathfrak{X}(M)$  on  $M$ .

In fact, Eq. (2.114) defines an anti-homomorphism of Lie algebras, specifically,

$$\begin{aligned} X^{aA+bB} &= aX^A + bX^B \\ [X^A, X^B] &= X^{-[A,B]} \end{aligned} \quad (2.115)$$

$\forall a, b \in \mathbb{R}, A, B \in \mathfrak{g}$ . Linearity follows because  $X_m^A = \Phi^m_* A$ , is the pushforward of a smooth map  $\Phi^m : G \rightarrow M$  defined by  $\Phi^m(g) = \Phi(g, m)$ . To see the second condition, note that

$$\begin{aligned}
X^{\text{Ad}_g A}(m) &= \left. \frac{d}{ds} \right|_{s=0} \Phi(g \exp(sA) g^{-1}, m) \\
&= \left. \frac{d}{ds} \right|_{s=0} \Phi_g \circ \Phi_{\exp(sA)} \circ \Phi_{g^{-1}}(m) \\
&= \Phi_{g_*} X_{\Phi_{g^{-1}}(m)}^A \\
&= (\Phi_{g^{-1}}^* X^A)(m)
\end{aligned} \tag{2.116}$$

where the first line follows from Eqs. (2.101) and (2.106), the second from the definition of a group action, the third by the chain rule, and the last by the definition of pullback for a vector, as in Eq. (2.73). Now setting  $g = \exp(tB)$  and differentiating with  $\left. \frac{d}{dt} \right|_{t=0}$ , the left hand side, by linearity and Eq. (2.111), becomes  $X^{\text{ad}_B A}$ , while the right hand side becomes  $\mathcal{L}_{X^{-B}} X^A = [X^{-B}, X^A]$ . Therefore,  $X^{[B, A]} = -[X^B, X^A]$ , as desired.

# 3

## Geometry and Symmetry II: Dynamical Systems

Having reviewed some fundamentals of geometry and symmetry groups in Chapter 2, this chapter will now extend these fundamentals toward the characterization of dynamical systems.

As its two driving sources, this chapter primarily follows Marsden and Ratiu [45] in its description of Hamiltonian dynamical systems, and Olver [53] in its description of symmetries in variational systems. Beyond the choice of presentation, no claim of originality is made in this chapter.

### 3.1 Hamiltonian formalism

Symmetries and conservation laws find a beautiful geometric expression in the Hamiltonian formalism for dynamical systems. Largely following Marsden and Ratiu [45], this section reviews relevant aspects of symplectic and Poisson geometry, before describing the momentum map—the Hamiltonian manifestation of Noether’s theorems. Consequences of the momentum map, including Poisson reduction [57, 58] and Lie-Poisson structure, are also discussed. A demonstration of this formalism is then

explored in a tangible Hamiltonian system, following the treatment of the Vlasov-Maxwell system in Marsden and Weinstein [59].

### 3.1.1 Symplectic manifolds

A *symplectic manifold*  $(M, \Omega)$  is a smooth manifold  $M$  equipped with a closed, nondegenerate 2-form  $\Omega \in \Lambda^2(M)$  called the *symplectic form*. Such a 2-form endows  $M$  with a rich structure that beautifully characterizes physical systems.<sup>(\*)</sup>

The paradigmatic example (or class of examples) of a symplectic manifold is the cotangent bundle of an arbitrary smooth manifold. In the context of Hamiltonian mechanics, a manifold  $Q$  can be defined to represent the *configuration space* of a system. In such a case, dynamics will be described on *phase space* defined as the cotangent bundle  $T^*Q$ , endowed with a natural symplectic structure. In particular, given local coordinates  $(q^1, \dots, q^n)$  on  $Q$ , a basis for  $T_q^*Q$  is given by  $(dq^1, \dots, dq^n)$ , so that any  $\alpha \in T_q^*Q$  can be expanded as  $\alpha = p_i dq^i$ . This induces a local coordinatization  $(q^1, \dots, q^n, p_1, \dots, p_n)$  for the  $2n$ -dimensional manifold  $T^*Q$ . The *canonical symplectic form*  $\Omega \in \Lambda^2(T^*Q)$  on  $T^*Q$  is then defined by

$$\Omega = dq^i \wedge dp_i, \tag{3.1}$$

which is immediately seen to be a closed, nondegenerate 2-form.<sup>(\*\*)</sup> This coordi-

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<sup>(\*)</sup> Symplectic manifolds are a superb example of the “unreasonable effectiveness of mathematics” [60].

<sup>(\*\*)</sup> Although  $\Omega$  appears to be coordinate-dependent in this construction, it can be more geometrically (if more abstractly) derived by defining a *tautological 1-form*  $\theta \in \Lambda^1(T^*Q)$  pointwise at each  $\beta \in T^*Q$  as

$$\theta_\beta(X) = (\pi_* X) \lrcorner \beta. \tag{3.2}$$

Here,  $X \in T_\beta(T^*Q)$  is a tangent vector at  $\beta$  and  $\pi : T^*Q \rightarrow Q$  is the cotangent bundle projection. In the local coordinate construction,  $\theta_p = pdq$  for  $p \in \pi^{-1}(q)$ . The canonical symplectic form is then defined by

$$\Omega = -d\theta. \tag{3.3}$$

In general, any symplectic manifold with an exact symplectic form  $\Omega$  is called *exact symplectic*.

natization of a symplectic 2-form is called *Darboux coordinates*, or *canonical form*. In fact, by *Darboux's theorem*, at any point  $m$  of an arbitrary symplectic manifold  $M$ , local coordinates can always be constructed so that  $\Omega$  is in canonical form on a neighborhood of  $m$ .

Because  $\Omega$  is nondegenerate, it induces a bijection between vector fields and 1-forms. In particular, given a 1-form  $\alpha_i$  in local coordinates, a vector field  $X^j$  can always be found such that  $\Omega_{ij}X^j = \alpha_i$  since  $\Omega_{ij}$  is invertible.<sup>(\*)</sup> Therefore,  $\forall H \in C^\infty(M)$ , there corresponds to the exact 1-form  $dH$  a vector field—denoted  $X_H$ —satisfying

$$\Omega(X_H, \cdot) = dH. \tag{3.4}$$

Such a vector field, for which  $\iota_{X_H}\Omega = dH$  is *exact*, is said to be *Hamiltonian*. Similarly, a vector field  $X$  for which  $\iota_X\Omega$  is *closed* is said to be *symplectic* (or *locally Hamiltonian*). All Hamiltonian vector fields are, therefore, symplectic.

The reason for this nomenclature is that, on a symplectic manifold, Hamiltonian dynamics are generated by the flow of a vector field  $X_H$  corresponding to a Hamiltonian  $H$ . In particular, *Hamilton's equations* for the evolution of a dynamical system are given in local coordinates  $\{z^i\}$  by

$$\dot{z} = X_H(z). \tag{3.5}$$

Moreover, because closed forms are locally exact, a symplectic vector field corresponds to a ‘local Hamiltonian’ (not necessarily globally defined). As the first example of a conservation law in Hamiltonian dynamics, it is straightforward to see that  $H$  is

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<sup>(\*)</sup> This calculation uses Roger Penrose's *abstract index notation* [61], in which uncontracted tensor indices—rather than denoting individual components of a tensor in a fixed coordinate basis—act as ‘placeholders’ that indicate the tensor type.

conserved along the flow of  $X_H$ , since by Eq. (2.73)

$$\begin{aligned} \left. \frac{d}{ds} \right|_{s=0} \exp(sX_H)^* H &= \mathcal{L}_{X_H} H = \iota_{X_H}(\mathrm{d}H) + \mathrm{d}\iota_{X_H} H \\ &= \iota_{X_H} \iota_{X_H} \Omega \\ &= 0 \end{aligned} \tag{3.6}$$

by the antisymmetry of  $\Omega$ . Generally, this fact corresponds to the conservation of energy.

The simple harmonic oscillator with Hamiltonian  $H = \frac{1}{2}(q^2 + p^2)$  provides a straightforward example to illustrate this formalism. Its phase space is coordinatized by  $\{(q, p)\} = \mathbb{R}^2$ , inducing the coordinate basis for the tangent space  $E = (\frac{\partial}{\partial q}, \frac{\partial}{\partial p})$ . In a matrix notation such that  $\Omega(X, Y) = X^T \Omega Y$ , therefore, the canonical symplectic form is expressed in the basis  $E$  as

$$\Omega = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}. \tag{3.7}$$

Since  $\mathrm{d}H = q\mathrm{d}q + p\mathrm{d}p = [q \ p]$ , Eq. (3.4) implies that  $X_H = p\frac{\partial}{\partial q} - q\frac{\partial}{\partial p}$ . Eq. (3.5) then simply defines dynamics on phase space by

$$\begin{bmatrix} \dot{q} \\ \dot{p} \end{bmatrix} = \left( p\frac{\partial}{\partial q} - q\frac{\partial}{\partial p} \right) \begin{bmatrix} q \\ p \end{bmatrix} = \begin{bmatrix} p \\ -q \end{bmatrix} \tag{3.8}$$

—the expected dynamics of the simple harmonic oscillator. Furthermore, note that  $X_H(H) = 0$ , as desired.

A *canonical transformation* (sometimes, *symplectomorphism* or *symplectic map*) of  $M$  is any diffeomorphism  $\phi : M \rightarrow M$  that preserves the symplectic form, i.e.

$$\phi^* \Omega = \Omega. \tag{3.9}$$

Appropriately, a vector field  $X$  is symplectic (i.e.  $\iota_X\Omega$  is closed) if and only if its flow is a symplectomorphism (i.e.  $\exp(sX)^*\Omega = \Omega$ ). After all, using Eqs. (2.72)-(2.73),

$$\begin{aligned} \left. \frac{d}{ds} \right|_{s=0} \exp(sX)^*\Omega &= \mathcal{L}_X\Omega = d(\iota_X\Omega) + \iota_X(d\Omega) \\ &= 0. \end{aligned} \tag{3.10}$$

### 3.1.2 Poisson manifolds

A *Poisson manifold*  $(M, \{\cdot, \cdot\})$  is a smooth manifold  $M$  equipped with a *Poisson bracket*  $\{\cdot, \cdot\} : C^\infty(M) \times C^\infty(M) \rightarrow C^\infty(M)$ , defined such that

- (a)  $\{\cdot, \cdot\}$  is a Lie bracket on  $C^\infty(M)$ ; and
- (b)  $\{\cdot, \cdot\}$  is a derivation in each factor, e.g.,

$$\{FG, H\} = \{F, H\}G + F\{G, H\} \tag{3.11}$$

$$\forall F, G, H \in C^\infty(M).$$

The Poisson bracket defines a multiplication rule that renders  $C^\infty(M)$  an algebra, known as the *Poisson algebra*.

An important example of a Poisson manifold is a symplectic manifold. In particular,  $(M, \Omega)$  is a Poisson manifold with bracket

$$\{F, G\}_\Omega = \Omega(X_F, X_G). \tag{3.12}$$

Using  $d\Omega = 0$ , it can be readily confirmed that Eq. (3.12) defines a Poisson bracket. It is instructive to think of Poisson manifolds, then, as a sometimes-degenerate generalization of symplectic manifolds.

The intuition for Hamiltonian dynamics on a Poisson manifold can be usefully

extended from the symplectic setting. Note that, by definition of the Poisson bracket

$$\{\cdot, F\} : C^\infty(M) \rightarrow C^\infty(M) \quad (3.13)$$

is a derivation on  $C^\infty(M) \forall F \in C^\infty(M)$ . As noted in the discussion following Eq. (2.31), the operator  $\{\cdot, F\}$  therefore corresponds to a vector field on  $M$ . The notion of a Hamiltonian vector field  $X_F$  on a symplectic manifold—wherein  $\iota_{X_F}\Omega = dF$ —is extended to the Poisson setting by defining the set of *Hamiltonian vectors on a Poisson manifold*  $(M, \{\cdot, \cdot\})$ ,

$$\mathfrak{X}_{\text{Ham}}(M) = \left\{ X_F \in \mathfrak{X}(M) \mid \exists F \in C^\infty(M) \text{ s.t. } X_F = \{\cdot, F\} \right\}. \quad (3.14)$$

Here,  $X_F = \{\cdot, F\}$  are equated as derivations on  $M$ . Note, this definition of  $\mathfrak{X}_{\text{Ham}}(M)$  is consistent with the notion of a Hamiltonian vector field on a symplectic manifold since, for a Poisson manifold  $(M, \{\cdot, \cdot\}_\Omega)$  defined by Eq. (3.12),

$$\{G, F\}_\Omega = \iota_{X_F}\iota_{X_G}\Omega = \iota_{X_F}dG = X_F(G) \quad \forall G \in C^\infty(M). \quad (3.15)$$

Because  $X_H = \{\cdot, H\}$ , the Hamiltonian evolution along the flow of  $X_H$  in the Poisson setting is achieved in local coordinates  $z^i$  by

$$\dot{z} = \{z, H\} \quad (3.16)$$

by analogy with Eq. (3.5). Therefore, the function  $H$  is called a *generating function* for the flow of the Hamiltonian vector field  $X_H$ . In particular,  $H$  generates the flow of  $X_H$  via the Poisson bracket.

One notes that, in the Poisson setting, it is even more immediate that  $H$  is conserved along its own flow, since  $\{H, H\} = 0$ . More generally, a function  $F$  is

constant along the flow generated by  $X_G$  if and only if  $\{F, G\} = 0$ .

On a Poisson manifold, there can exist any number of functions  $C \in C^\infty(M)$  satisfying

$$\{F, C\} = 0 \quad \forall F \in C^\infty(M). \quad (3.17)$$

Such functions are called *Casimirs*, denoted  $C_{\text{Cas}}^\infty(M) \subset C^\infty(M)$ . They can be viewed as the commuting center of the Poisson algebra  $C^\infty(M)$ , and they characterize the degeneracy of a Poisson manifold. Clearly, the Hamiltonian vector field associated to any Casimir  $C \in C_{\text{Cas}}^\infty(M)$  vanishes, i.e.  $X_C = 0$ . Whereas the only Casimirs on a symplectic manifold are constant functions— $F_0$  for which  $dF_0 = 0$ —the Casimirs of a Poisson manifold are, in general, nontrivial.

Note that because the Poisson bracket is bilinear, the Hamiltonian vector fields  $\mathfrak{X}_{\text{Ham}}(M)$  are linear in  $C^\infty(M)$ . In particular,

$$X_F + X_G = \{\cdot, F\} + \{\cdot, G\} = \{\cdot, F + G\} = X_{F+G}. \quad (3.18)$$

However, the existence of Casimirs spoils any one-to-one correspondence between  $\mathfrak{X}_{\text{Ham}}(M)$  and  $C^\infty(M)$ . In particular, for any Casimir  $C$ ,  $X_F = X_{F+C}$ .

Lastly, canonical transformations can be characterized on Poisson manifolds as those diffeomorphisms  $\phi : M \rightarrow M$  preserving the Poisson bracket, such that

$$\{\phi^*F, \phi^*G\} = \phi^*\{F, G\} \quad (3.19)$$

$\forall F, G \in C^\infty(M)$ . (Using Eqs. (3.9) and (3.12), it is straightforward to show that this definition coincides with the notion of a symplectomorphism for  $M$  symplectic.)

For  $\phi$  generated by the flow of a vector field  $X$ , the pullback  $\phi^*$  may be differentiated as in Eq. (2.72) to yield the Lie derivative with respect to  $X$ , such that Eq. (3.19)

infinitesimally becomes

$$\{X(F), G\} + \{F, X(G)\} = X(\{F, G\}). \quad (3.20)$$

It immediately follows from the Jacobi identity that Eq. (3.20) holds for any Hamiltonian vector field  $X = X_H = \{\cdot, H\}$ . Therefore, just as Hamiltonian vector fields generate canonical transformations on symplectic manifolds, they do so on Poisson manifolds as well. A vector field satisfying Eq. (3.20) is called an *infinitesimal Poisson automorphism*, a class of vector fields denoted  $\mathfrak{X}_{\text{IPA}}(M)$ . Therefore,

$$\mathfrak{X}_{\text{Ham}}(M) \subset \mathfrak{X}_{\text{IPA}}(M) \subset \mathfrak{X}(M). \quad (3.21)$$

### 3.1.3 Momentum maps

Consider a canonical group action of a Lie group  $G$  on a Poisson manifold  $(M, \{\cdot, \cdot\})$ , that is,

$$\Phi : G \times M \rightarrow M \quad \text{s.t.} \quad \{\Phi_g^* F, \Phi_g^* H\} = \Phi_g^* \{F, H\} \quad \forall g \in G, \quad (3.22)$$

as defined in Eqs. (2.113) and (3.19). Each Lie algebra element  $A \in \mathfrak{g}$  induces an infinitesimal generator  $X^A \in \mathfrak{X}(M)$  of  $\Phi$ , namely  $X^A = \left. \frac{d}{ds} \right|_{s=0} \Phi_{\exp(sA)}$ —as described in Eq. (2.114). (To emphasize notation, a subscripted  $X_F$  indicates a Hamiltonian vector field—with  $F \in C^\infty(M)$ —while a superscripted  $X^A$  denotes an infinitesimal generator of a Lie group action—with  $A \in \mathfrak{g}$ .)

Since the group action is canonical, its generators satisfy Eq. (3.20), that is,  $X^A \in \mathfrak{X}_{\text{IPA}}(M) \forall A \in \mathfrak{g}$ . Moreover, as noted in Eq. (2.115), the induced vector fields

on  $M$  are linear in the Lie algebra, such that

$$X^{A+B} = X^A + X^B. \quad (3.23)$$

Since  $\mathfrak{X}_{\text{Ham}}(M) \subset \mathfrak{X}_{\text{IPA}}(M)$ , one might hope that the generator of a canonical group action  $X^A \in \mathfrak{X}_{\text{IPA}}(M)$  is also a Hamiltonian vector field. While this will not always be the case, identifying the generator of a group action as a Hamiltonian vector field powerfully clarifies its relationship with the dynamics of a physical system. This characterization of a canonical group action is called the *momentum map* [44–46].

In particular, suppose  $X^A \in \mathfrak{X}_{\text{Ham}}(M) \forall A \in \mathfrak{g}$ . Then there exists some generating function  $J(A) \in C^\infty(M)$  for each  $A \in \mathfrak{g}$ , such that

$$X^A = X_{J(A)} = \{\cdot, J(A)\}. \quad (3.24)$$

Such a map

$$J : \mathfrak{g} \rightarrow C^\infty(M) \quad (3.25)$$

discovers a generating function  $J(A)$  for each infinitesimal generator  $X^A$  of the group action  $\Phi$ . This is the essential character of the momentum map—it assigns to every Lie algebra element  $A \in \mathfrak{g}$  of the group action a *generating function* on  $M$  that generates its flow. Just as a Hamiltonian  $H \in C^\infty(M)$  is a function on phase space, whose flows determine a system’s evolution in time,  $J(A)$  is a function on phase space, whose flows implement group transformations of the phase space corresponding to  $\Phi$ .

Note that, since the infinitesimal generators  $X^A$  are linear in the Lie algebra (as in Eq. (3.23)),  $J$ , too, if it exists, must be a linear function of  $\mathfrak{g}$ , such that  $J : \mathfrak{g} \rightarrow C^\infty(M)$  is a linear map. The *momentum map*  $\mu$  is an object that makes the linearity of  $J$  somewhat more apparent. In particular, the momentum map  $\mu$  is

defined as the map

$$\begin{aligned} \mu : M &\rightarrow \mathfrak{g}^* \\ m &\mapsto \mu(m) \quad \text{s.t.} \quad \langle \mu(m), A \rangle = J(A)|_m. \end{aligned} \tag{3.26}$$

Here,  $\langle \cdot, \cdot \rangle : \mathfrak{g}^* \times \mathfrak{g} \rightarrow \mathbb{R}$  denotes the natural bilinear pairing between elements of  $\mathfrak{g}$  and its dual  $\mathfrak{g}^*$ . Thus, the momentum map  $\mu$  assigns a dual element  $\mu(m) \in \mathfrak{g}^*$  to each point of the manifold  $M$ , such that, when  $\mu$  is everywhere paired with a fixed element  $A \in \mathfrak{g}$  of the Lie algebra, the resulting function  $J(A)$  on  $M$  is a generating function of  $X^A$ —that is,  $X^A = \{\cdot, J(A)\}$ .

For connected Lie groups, the dual pictures of the momentum map as

- $J : \mathfrak{g} \rightarrow C^\infty(M)$ , a linear map from Lie algebra elements to their generating functions on  $M$ , or
- $\mu : M \rightarrow \mathfrak{g}^*$ , a  $\mathfrak{g}^*$ -valued function on  $M$  that everywhere ‘eats’ a fixed Lie algebra element and returns a generating function on  $M$

are equivalent to one another. Although  $J$  offers a somewhat more intuitive framing of the momentum map, as technical objects  $\mu$  and  $J$  are both convenient.

So far, the group action  $\Phi$  has simply been described as some family of canonical transformations of  $M$  associated with a Lie group  $G$ . A group action  $\Phi$  is further said to be a *symmetry* of a Hamiltonian system on  $M$ , however, when the Hamiltonian  $H$  is invariant under its transformations. In particular,  $\Phi$  is called a *symmetry of  $H$*  (and  $H$  is said to be  *$G$ -invariant*) when

$$\Phi_g^* H = H \quad \forall g \in G. \tag{3.27}$$

Note that the momentum map has been defined independent of the Hamiltonian, and its characterization of a group action in terms of generating functions is not

affected by the symmetry characteristics of the Hamiltonian.  $\mu$  is simply a kinematic (as opposed to dynamic) object determined by  $\Phi$  and the Poisson manifold  $M$  [62]. Nevertheless, the full implications of the momentum map are revealed when one considers how  $\mu$  behaves in the context of Hamiltonian dynamics.

In particular, by setting  $g = \exp(tA)$  in Eq. (3.27) and differentiating ‘with respect to  $g$ ’, one of course finds that an  $H$  invariant under  $\Phi$  is infinitesimally invariant under its generators. (This fact will also be critical in the characterization of Lagrangian symmetries described in Section 3.2.) Indeed, differentiating Eq. (3.27) yields

$$X^A(H) = 0. \tag{3.28}$$

Given a momentum map for this group action, which associates generating functions to the infinitesimal generator  $X^A$ , it is seen that

$$\begin{aligned} H = \Phi_{\exp(tA)}^* H \quad \Rightarrow \quad 0 = X^A(H) &= \{H, J(A)\} = -\{J(A), H\} \\ &= -\dot{J}(A) = -\frac{d}{dt}\langle\mu, A\rangle = -\langle\dot{\mu}, A\rangle. \end{aligned} \tag{3.29}$$

This result is the Hamiltonian counterpart to Noether’s first theorem. For each symmetry of  $H$  (that is, for each linearly independent  $A \in \mathfrak{g}$ ), there exists a unique first integral of the system—i.e.  $J(A) = \langle\mu, A\rangle$ . Thus,  $\mu$  determines  $\mathbf{dim}[G]$  conservation laws in a Hamiltonian system symmetric under a canonical group action of the Lie group  $G$ . Since  $\frac{d}{dt}\langle\mu, A\rangle = 0$  holds for arbitrary  $A \in \mathfrak{g}$ , the entire momentum map is invariant under the flow of  $H$ , that is

$$\dot{\mu} = \{\mu, H\} = 0. \tag{3.30}$$

It is worth highlighting that for each  $A \in \mathfrak{g}$ , the function  $J(A)$  is both a generating

function of the transformation  $\Phi_{\exp(sA)}$  and the conserved quantity associated with it. This double-duty is a feature more familiar, perhaps, in a quantum mechanical setting. There, a charge operator  $\hat{Q}$  is not just a conserved quantity, satisfying  $[\hat{Q}, \hat{H}] = 0$ , but also the *generator* of gauge transformations associated with charge, e.g. for a state of charge  $q$ ,  $\hat{Q}|\psi_q\rangle = q|\psi_q\rangle$  and  $e^{i\theta\hat{Q}}|\psi_q\rangle = e^{i\theta q}|\psi_q\rangle$ . The generator of symmetry and the conserved quantity are one and the same. In this sense, the momentum map is a feature of classical mechanics that draws near to its quantum counterpart.

### When does a momentum map exist?

As one might surmise from the nested subsets  $\mathfrak{X}_{\text{Ham}}(M) \subset \mathfrak{X}_{\text{IPA}}(M) \subset \mathfrak{X}(M)$  of Eq. (3.21), it is not always the case that a canonical Lie group action has a corresponding momentum map. It is therefore sensible to ask what conditions guarantee the existence of a momentum map.

An algebraic point of view [45] will assist in answering this question. Assuming that a canonical group action of the Lie group  $G$  is defined on the Poisson manifold  $M$ , consider the following diagram:

$$\begin{array}{ccccccc}
 0 & \longrightarrow & C_{\text{Cas}}^\infty(M) & \xrightarrow{\iota} & C^\infty(M) & \xrightarrow{\mathcal{H}: F \mapsto X_F} & \mathfrak{X}_{\text{IPA}}(M) & \xrightarrow{\pi} & \mathfrak{X}_{\text{IPA}}(M)/\mathfrak{X}_{\text{Ham}}(M) & \longrightarrow & 0 \\
 & & & & & & \swarrow J & & \nearrow \rho: A \mapsto X^A & & \\
 & & & & & & \mathfrak{g} & & & & 
 \end{array}$$

Figure 3.1: The upper row of this diagram is an exact sequence, (i.e.,  $\mathbf{Im}f_i = \mathbf{Ker}f_{i+1}$  as defined in Section 2.3.7.)  $\iota$  denotes the inclusion of Casimir functions, and  $\pi$  denotes the projection that annihilates Hamiltonian vector fields. If a map  $J$  exists which renders the above a commuting diagram, then  $J$  defines a momentum map. Since the upper row is exact, such a  $J$  exists if and only if  $\pi \circ \rho = 0$ .

$\rho$  is well-defined in Fig. 3.1 because the group action is assumed canonical. Since the upper row is an exact sequence, a map  $J$  exists that makes the diagram commute

if and only if

$$\pi \circ \rho = 0. \quad (3.31)$$

One sufficient criterion for the existence of the momentum map, then, is certainly given by  $\pi = 0$ , or equivalently,  $\mathfrak{X}_{\text{IPA}}(M) = \mathfrak{X}_{\text{Ham}}(M)$ . Consider, for example, the following two cases:

(1) When  $M$  is symplectic, recall that

$$X \in \mathfrak{X}_{\text{IPA}}(M) \Rightarrow X \text{ symplectic} \Rightarrow d\iota_X \Omega = 0 \text{ (closed)} \quad (3.32)$$

$$X = X_F \in \mathfrak{X}_{\text{Ham}}(M) \Rightarrow X \text{ Hamiltonian} \Rightarrow \iota_X \Omega = dF \text{ (exact)}. \quad (3.33)$$

Therefore, for  $M$  symplectic, the condition  $\pi = 0$  is equivalent to the vanishing of the first cohomology group,  $H^1(M)$ , as defined in Eq. (2.76). Since  $H^1(\mathbb{R}^2) = 0$ , for example, any canonical group action on a single particle phase space has an associated momentum map.

(2) As another example, if  $M$  is exact symplectic—i.e.,  $\Omega = -d\theta$  for some  $\theta \in \Lambda^1(M)$  as in Eq. (3.3)—and  $\theta$  is invariant under the canonical group action—i.e.  $\mathcal{L}_{X^A}\theta = 0$ —then a momentum map exists. After all, given  $X^A \in \mathfrak{X}_{\text{IPA}}(M)$  on an exact symplectic manifold  $(M, \Omega)$ ,

$$\iota_{X^A} \Omega = -\iota_{X^A} d\theta = -(\mathcal{L}_{X^A} - d\iota_{X^A})\theta = d\iota_{X^A}\theta. \quad (3.34)$$

Thus,  $X^A \in \mathfrak{X}_{\text{Ham}}(M)$  and  $\pi = 0$  again. Indeed, from Eq. (3.34) it is seen that  $J(A) = \iota_{X^A}\theta$  yields the desired momentum map.

### 3.1.4 Further applications of the momentum map

#### Poisson reduction

The symmetry of a Hamiltonian system often renders various points of phase space physically redundant with one another. One wonders, therefore, if, while somehow preserving the Poisson structure of phase space, one can reduce the phase space to a submanifold that eliminates this redundancy. This is the program of *Poisson reduction* [57, 58, 63].

By the quotient manifold theorem, for any smooth manifold  $M$  with a Lie group action  $\Phi : G \times M \rightarrow M$  that is

- *free*: if for any  $m \in M$ ,  $\Phi_g(m) = m$ , then  $g = \mathbb{1}$ ; and
- *proper*: preimages of compact sets are compact under  $(g, m) \mapsto (m, \Phi_g(m))$

then the quotient map  $\pi : M \rightarrow M/G$  is a smooth submersion ( $\pi_*$  is everywhere surjective) and the *quotient manifold*  $M/G$  is smooth. Moreover, if  $(M, \{\cdot, \cdot\})$  is Poisson and the group action is canonical, then  $M/G$  is also equipped with a Poisson bracket  $\{\cdot, \cdot\}^{M/G}$  uniquely determined by

$$\pi^*\{F, K\}^{M/G} = \{\pi^*F, \pi^*K\} \quad \forall F, K \in C^\infty(M/G). \quad (3.35)$$

Given a  $G$ -invariant Hamiltonian  $H \in C^\infty(M)$ , its flow on  $M$  generated by  $X_H$  commutes with the group action, so that  $\pi$  induces a Hamiltonian flow on the reduced Poisson manifold  $(M/G, \{\cdot, \cdot\}^{M/G})$  corresponding to the *reduced Hamiltonian*  $[H]$  satisfying  $\pi^*[H] = H$ .

There is a more specialized approach to Poisson reduction for a symmetric Hamiltonian system whose group action admits a momentum map  $\mu$ . In particular, since the momentum map  $\mu$  is preserved along the flow of  $H$ , much of the Poisson manifold  $M$ —specifically, every point where  $\mu$  takes a different value—goes ‘unused’ in its evolution. In this case, Poisson reduction can be carried out by first restricting the

manifold  $M$  to level sets of  $\mu$ , and then forming a quotient manifold, as above. This proceeds as follows [58].

Suppose the canonical, free, proper group action  $\Phi$  above has a momentum map  $\mu$  that is *group-equivariant*—i.e. it satisfies

$$\mu \circ \Phi_g = \text{Ad}_{g^{-1}}^* \circ \mu. \quad (3.36)$$

Then consider the preimage of a regular value  $\alpha \in \mathfrak{g}^*$  under  $\mu : M \rightarrow \mathfrak{g}^*$ , i.e., the level set  $\mu^{-1}(\alpha) \subset M$ . (Here, a *regular value* is any point  $\alpha \in \mathfrak{g}^*$  such that  $T_m\mu$  is surjective  $\forall m \in \mu^{-1}(\alpha)$ .) Denote by  $G_\alpha \subset G$  the isotropy subgroup of  $G$  that leaves  $\alpha$  invariant under the coadjoint action. (At  $\alpha = 0$ ,  $G_\alpha = G$  since  $\text{Ad}_{g^{-1}}^*$  is linear.) Then for a regular value  $\alpha \in \mathfrak{g}^*$  of  $\mu$ , the Poisson reduction of  $M$  is the unique quotient map  $\pi : (\mu^{-1}(\alpha), \{\cdot, \cdot\}_M) \rightarrow (\mu^{-1}(\alpha)/G_\alpha, \{\cdot, \cdot\}^{\mu^{-1}(\alpha)/G_\alpha})$  from the level set of  $\mu$  satisfying the counterpart of Eq. (3.35), i.e.,  $\pi^*\{F, K\}^{\mu^{-1}(\alpha)/G_\alpha} = \{\pi^*F, \pi^*K\}$ .

In particular, Poisson reduction first considers just the level set  $\mu^{-1}(\alpha)$  of  $M$  and then mods out by the group action to find the quotient manifold  $\mu^{-1}(\alpha)/G_\alpha$ , taking just a ‘slice’ of  $\mu^{-1}(\alpha)$  under the action of  $G_\alpha$ . Note that, because  $\mu$  is equivariant in the sense of Eq. (3.36) and because  $G_\alpha$  leaves the right hand side of Eq. (3.36) constant,  $\mu^{-1}(\alpha)$  is preserved by  $G_\alpha$  and  $\mu^{-1}(\alpha)/G_\alpha$  is well defined. The reduced manifold  $\mu^{-1}(\alpha)/G_\alpha$  is again a Poisson manifold.

## Lie-Poisson structure

A particularly natural Poisson structure, which arises via Poisson reduction, is the *Lie-Poisson structure*. The Lie-Poisson structure underpins a wide class of physical systems, ranging from rigid bodies to perfect fluids [64], whose dynamics are closely associated with transformation groups.

Lie-Poisson structures often arise when the configuration space of a physical sys-

tem is described as a Lie group  $G$ . A canonical example is given by a rigid body with one fixed point, whose configurations can be uniquely described by a rotation of the body with respect to some reference configuration; the configuration space of the system is therefore  $SO(3)$ . The Lagrangian of a system with configuration space  $G$  is defined on the tangent bundle  $TG$ —just as the Lagrangian of a single particle with configuration space  $Q = \{q\}$  is defined on  $TQ = \{(q, \dot{q})\}$ .  $TG$  can then be mapped by a Legendre transform to a Hamiltonian system on  $T^*G$ , the cotangent bundle of the Lie group  $G$ , endowed with the usual canonical symplectic structure.

At this point, the symmetry of the system under transformations by  $G$  can be modded out by the process of Poisson reduction. (In the aforementioned case of the rigid body, for example, note that the reference configuration is arbitrarily chosen. There is a “global gauge freedom,” therefore, in associating configurations with  $SO(3)$  rotations.) In this case, the momentum map facilitating the reduction is associated with the group action of left translation,  $\ell_g : G \rightarrow G$ , which induces a group action on  $T^*G$  (defined by the *cotangent lift*—the dual map to the pushforward).

Since the cotangent bundle  $T^*G$  of a Lie group is isomorphic to the trivial bundle  $G \times \mathfrak{g}^*$  (in the same way that  $\mathfrak{g}$  is isomorphic to left-invariant vector fields on  $G$ ), it is readily shown that  $T^*G/G \cong \mathfrak{g}^*$ , the dual Lie algebra of  $G$ . By this so-called *Lie-Poisson reduction* [45], a  $G$ -invariant system defined on  $T^*G$  can be described by its ‘reduced’ dynamics on  $\mathfrak{g}^*$ .

The canonical symplectic structure on  $T^*G$  is thereby reduced to a *Lie-Poisson bracket* on  $\mathfrak{g}^*$ . In particular,  $\mathfrak{g}^*$  is defined to be a Poisson manifold with Lie-Poisson bracket  $\{\cdot, \cdot\}_- : C^\infty(\mathfrak{g}^*) \times C^\infty(\mathfrak{g}^*) \rightarrow C^\infty(\mathfrak{g}^*)$  defined pointwise  $\forall \alpha \in \mathfrak{g}^*$  as follows:

$$\{F, H\}_-(\alpha) = - \left\langle \alpha, \left[ \frac{\delta F}{\delta \alpha}, \frac{\delta H}{\delta \alpha} \right] \right\rangle \quad (3.37)$$

$\forall F, H \in C^\infty(\mathfrak{g}^*)$ , the set of smooth functions on  $\mathfrak{g}^*$ . Here,  $[\cdot, \cdot]$  is the usual Lie bracket

of  $\mathfrak{g}$  and  $\langle \cdot, \cdot \rangle$  is the bilinear pairing of  $\mathfrak{g}^*$  and  $\mathfrak{g}$ .  $\delta F/\delta\alpha \in \mathfrak{g}$  denotes the unique element of  $\mathfrak{g}$  such that

$$dF(\alpha) \cdot \beta = \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} F(\alpha + \epsilon\beta) = \left\langle \beta, \frac{\delta F}{\delta\alpha} \right\rangle \quad (3.38)$$

$\forall \beta \in \mathfrak{g}^*$ , where  $dF(\alpha)$  is the differential of  $F$  at  $\alpha$ . It is readily seen that Eq. (3.37) satisfies the properties of a Poisson bracket: It is antisymmetric, bilinear, and satisfies the Leibniz and Jacobi identities. (The negative sign in Eq. (3.37) is the result of pursuing a Poisson reduction corresponding to the left translation group action on the configuration space  $G$ . Right translation would induce the opposite sign. In the case of a rigid body, this distinction gives rise to its two descriptions in body or spatial coordinates, for example.)

### 3.1.5 Example: The Vlasov-Maxwell system

The elements of Poisson geometry that have been developed in the last few sections will now be applied toward the analysis of the Hamiltonian Vlasov-Maxwell system. This treatment prepares for the analysis of discrete Vlasov-Maxwell systems in Chapter 5.

The Poisson structure of the Vlasov-Maxwell system was derived in Morrison [65] and independently in Iwinski and Turski [66], and later presented with a correction in Marsden and Weinstein [59], with a limitation to this correction emphasized in [67] by a direct proof of the Jacobi identity. Closely following this last reference, this section reviews the Poisson reduction [57, 58] of the Vlasov-Maxwell system, which ‘spends’ the system’s gauge symmetries in order to eliminate their associated redundant (gauge) degrees of freedom. This Poisson reduction is achieved via the momentum map, which in turn determines the local charge conservation law of the Vlasov-Maxwell system. The following section serves as a concise pedagogical sum-

mary of [59], with additional discussion relevant to the more recent plasma physics literature.

As a starting point, consider the Poisson bracket of Marsden and Weinstein [59] for the Vlasov-Maxwell system defined over the spatial domain  $\mathbb{R}^3$ ,

$$\{\{F, G\}\}[f, \mathbf{A}, \mathbf{Y}] = \int d\mathbf{x}d\mathbf{p} f \left\{ \frac{\delta F}{\delta f}, \frac{\delta G}{\delta f} \right\}_{\mathbf{x}\mathbf{p}} + \int d\mathbf{x} \left( \frac{\delta F}{\delta \mathbf{A}} \cdot \frac{\delta G}{\delta \mathbf{Y}} - \frac{\delta G}{\delta \mathbf{A}} \cdot \frac{\delta F}{\delta \mathbf{Y}} \right) \quad (3.39)$$

with time evolution defined by the Hamiltonian

$$H[f, \mathbf{A}, \mathbf{Y}] = \frac{1}{2} \int f \cdot |\mathbf{p} - \mathbf{A}|^2 d\mathbf{x}d\mathbf{p} + \frac{1}{2} \int [|\mathbf{Y}|^2 + |\nabla \times \mathbf{A}|^2] d\mathbf{x}. \quad (3.40)$$

Here,  $F$  and  $G$  represent arbitrary functionals of the distribution function  $f(\mathbf{x}, \mathbf{p})$ , the 3-component vector potential  $\mathbf{A}(\mathbf{x})$  and its conjugate momentum  $\mathbf{Y}(\mathbf{x})$ . As shall be seen momentarily,  $\mathbf{Y}$  can be readily identified as negative the electric field strength—(i.e.,  $\mathbf{Y} = -\mathbf{E}$ ). This system is rendered in the temporal gauge, wherein the electric potential satisfies  $\phi(\mathbf{x}) = 0$ . As in Marsden and Weinstein [59], the Poisson bracket in Eq. (3.39) is denoted  $\{\{\cdot, \cdot\}\}$  merely to distinguish it from other Poisson structures.

The  $\int d\mathbf{x}d\mathbf{p} f \{\delta_f \cdot, \delta_f \cdot\}_{\mathbf{x}\mathbf{p}}$  operator in the first line of Eq. (3.39) is a Lie-Poisson bracket [45], which defines a Poisson structure for functions on a dual Lie algebra  $\mathfrak{g}^*$ . In the present context, the Lie algebra  $\mathfrak{g}$  corresponds to infinitesimal transformations of  $(\mathbf{x}, \mathbf{p}) \cong \mathbb{R}^6$ , the position-momentum phase space. Such transformations can be regarded as Hamiltonian vector fields on  $\mathbb{R}^6$ , which map via anti-homomorphism to their corresponding generating functions, i.e.

$$[\mathbf{X}_h, \mathbf{X}_k] = -\mathbf{X}_{\{h, k\}_{\mathbf{x}\mathbf{p}}}. \quad (3.41)$$

The bracket  $\{\cdot, \cdot\}_{\mathbf{x}\mathbf{p}}$  therefore serves as a Lie bracket, defined pointwise on  $\mathbb{R}^6$

$$\{h, k\}_{\mathbf{x}\mathbf{p}} := \left( \partial_{\mathbf{x}} h \cdot \partial_{\mathbf{p}} k - \partial_{\mathbf{x}} k \cdot \partial_{\mathbf{p}} h \right). \quad (3.42)$$

The dual Lie algebra  $\mathfrak{g}^*$  is similarly identified by distribution densities on  $\mathbb{R}^6$ , which pair linearly to Hamiltonian functions via integration

$$\langle f, h \rangle := \int f h \, d\mathbf{x}d\mathbf{p} \quad (3.43)$$

for  $f \in \mathfrak{g}^*, h \in \mathfrak{g}$ .

In this way, the operator  $\int d\mathbf{x}d\mathbf{p} f \{\delta_{f\cdot}, \delta_{f\cdot}\}_{\mathbf{x}\mathbf{p}}$  comprising the first term of Eq. (3.39) is seen to be a Lie-Poisson bracket of the form in Eq. (3.37). The negative sign of Eq. (3.37) cancels with the negative sign of the anti-homomorphism of Eq. (3.41) to produce this operator.

The second term of Eq. (3.39) represents the electromagnetic ‘sector’ of the Poisson structure, and derives from the canonical symplectic structure on the cotangent space— $T^*Q = \{(\mathbf{A}, \mathbf{Y})\}$ —of the configuration space  $Q = \{\mathbf{A}\}$ . Therefore, the complete setting of the Vlasov-Maxwell system is a Poisson manifold, given by

$$M = \mathfrak{g}^* \times T^*Q \quad (3.44)$$

with its bracket defined in Eq. (3.39).

Now consider dynamics on this Poisson manifold  $M$ . To derive its Hamiltonian’s equation of motion, it is convenient to define functionals

$$F(\mathbf{u}) := \int d\mathbf{u}' F(\mathbf{u}') \delta(\mathbf{u} - \mathbf{u}') \quad (3.45)$$

for  $F \in \{f, \mathbf{A}, \mathbf{Y}\}$  as in [15], where  $\mathbf{u} = (\mathbf{x}, \mathbf{p})$  or  $\mathbf{u} = \mathbf{x}$ , as appropriate. Plugging

such functionals into Eqs. (3.39)-(3.40), one finds

$$\begin{aligned}
\dot{f}(\mathbf{x}, \mathbf{p}) &= \{\{f, H\}\} = -\left[\partial_{\mathbf{x}}f + \partial_{\mathbf{p}}f \cdot (\nabla \mathbf{A})\right] \cdot (\mathbf{p} - \mathbf{A}) \\
\dot{\mathbf{A}}(\mathbf{x}) &= \{\{\mathbf{A}, H\}\} = \mathbf{Y} \\
\dot{\mathbf{Y}}(\mathbf{x}) &= \{\{\mathbf{Y}, H\}\} = \int f \cdot (\mathbf{p} - \mathbf{A})d\mathbf{p} - \nabla \times \nabla \times \mathbf{A}.
\end{aligned} \tag{3.46}$$

Observe that  $\mathbf{Y}$  plays the role of  $-\mathbf{E}$ , as expected. For convenience, note that the familiar form of the Vlasov equation may be recovered from the first line of Eq. (3.46) by defining a distribution density  $\bar{f}$  on  $(\mathbf{x}, \mathbf{v})$  space where  $\mathbf{v} = \mathbf{p} - \mathbf{A}$ , i.e.

$$f(\mathbf{x}, \mathbf{p}) = \bar{f}(\mathbf{x}, \mathbf{p} - \mathbf{A}) = \bar{f}(\mathbf{x}, \mathbf{v}), \tag{3.47}$$

such that  $\partial_{\mathbf{x}}f = \partial_{\mathbf{x}}\bar{f} - (\nabla \mathbf{A}) \cdot \partial_{\mathbf{v}}\bar{f}$ ;  $\partial_{\mathbf{p}}f = \partial_{\mathbf{v}}\bar{f}$ ; and  $\dot{f} = \partial_t\bar{f} - \dot{\mathbf{A}} \cdot \partial_{\mathbf{v}}\bar{f}$ . Here,  $\nabla \equiv \partial_{\mathbf{x}}$  are used interchangeably, and the dyad convention

$$\mathbf{v} \cdot \mathbf{A}\mathbf{B} \cdot \mathbf{w} = v_i A_i B_j w_j \tag{3.48}$$

is used.

### Gauge symmetry and the momentum map

With Poisson and Hamiltonian structures in hand, one may now consider the gauge symmetry of the Vlasov-Maxwell system. Continuing to follow [59], a group action  $\Phi_\psi : M \rightarrow M$  may be defined on the Poisson manifold  $M = \mathfrak{g}^* \times T^*Q$  of the form

$$\Phi_\psi : (f, \mathbf{A}, \mathbf{Y}) \mapsto \left(f \circ \tau_\psi, \mathbf{A} - \nabla\psi, \mathbf{Y}\right), \tag{3.49}$$

where

$$\tau_\psi(\mathbf{x}, \mathbf{p}) := (\mathbf{x}, \mathbf{p} + \nabla\psi). \quad (3.50)$$

It is worth emphasizing that  $\Phi_\psi$  transforms  $f$ , and not  $\mathbf{p}$  itself. It is straightforward to check that  $\Phi_\psi$  is a *canonical group action*, i.e. that the Poisson bracket is preserved by the pullback of  $\Phi_\psi$ , namely  $\Phi_\psi^*\{\{F, G\}\} = \{\{\Phi_\psi^*F, \Phi_\psi^*G\}\}$ .

Such an arbitrary function  $\psi \in \mathcal{F}$  is defined as belonging to the abelian group  $\mathcal{F} := C^\infty(\mathbb{R}^3)$  of smooth functions on  $\mathbb{R}^3$ , with the group composition law of addition. Its Lie algebra  $\mathfrak{f}$  is also identifiable as the smooth functions on  $\mathbb{R}^3$ , while its dual  $\mathfrak{f}^*$  is the set of densities over  $\mathbb{R}^3$  that pair to elements of  $\mathfrak{f}$  via integration over  $\mathbb{R}^3$ —analogous to the  $\mathbb{R}^6$  integration of Eq. (3.43).

Now let  $\phi \in \mathfrak{f}$  denote an arbitrary Lie algebra element, such that  $\exp(\epsilon\phi) \in \mathcal{F} \forall \epsilon \in \mathbb{R}$ . By differentiating the group action  $\Phi_{\exp(\epsilon\phi)}$  on  $M$ , one may associate to any such  $\phi \in \mathfrak{f}$  the corresponding vector field  $X^\phi$  on  $M$ , namely

$$X^\phi := \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} \Phi_{\exp(\epsilon\phi)}. \quad (3.51)$$

The vector field  $X^\phi$  is therefore the infinitesimal generator of the group action on  $M$  corresponding to  $\phi \in \mathfrak{f}$ .

Since  $\Phi$  is a canonical group action on the Poisson manifold  $M$ , one may seek a corresponding momentum map  $\mu : M \rightarrow \mathfrak{f}^*$  satisfying

$$\{\{F, \langle \mu, \phi \rangle\}\} = X^\phi(F) \quad (3.52)$$

for arbitrary  $F \in C^\infty(M)$ . Here,  $X^\phi(F)$  is the Lie derivative of  $F$  along the vector field  $X^\phi$ . In particular, the momentum map  $\mu$  assigns a dual element of  $\mathfrak{f}^*$  to each point of  $M$  such that, when  $\mu$  is everywhere paired with an element  $\phi \in \mathfrak{f}$  of the Lie

algebra, the resulting function  $\langle \mu, \phi \rangle = J(\phi)$  on  $M$  is a generating function of the associated vector field  $X^\phi$ .

To find  $\mu$  for the Vlasov-Maxwell system of interest, first note that a single point  $m \in M = \mathfrak{g}^* \times T^*Q$  specifies  $(f, \mathbf{A}, \mathbf{Y})$  over the entire  $(\mathbf{x}, \mathbf{p})$  phase space. Given the group action defined in Eqs. (3.49)-(3.50), it is immediately seen that  $X^\phi = \frac{d}{d\epsilon} \Big|_{\epsilon=0} \Phi_{\exp(\epsilon\phi)}$  can be expressed as the following infinitesimal operator on  $M$  corresponding to  $\phi(\mathbf{x}) \in \mathfrak{f}$ :

$$\{\{\cdot, J(\phi)\}\} = \int d\mathbf{x}d\mathbf{p} \nabla\phi \cdot \frac{\partial f}{\partial \mathbf{p}} \frac{\delta}{\delta f} - \int d\mathbf{x} \nabla\phi \cdot \frac{\delta}{\delta \mathbf{A}}. \quad (3.53)$$

Upon inspection, it is evident that to generate the operator of Eq. (3.53), the Poisson bracket of Eq. (3.39) requires that  $\langle \mu(m), \phi \rangle = J(\phi)$  be given by

$$\langle \mu(m), \phi \rangle = \int d\mathbf{x} \left[ \int d\mathbf{p} f(\mathbf{x}, \mathbf{p}) + \nabla \cdot \mathbf{Y} \right] \phi(\mathbf{x}), \quad (3.54)$$

where  $\langle \cdot, \cdot \rangle = \int d\mathbf{x}$ . Therefore, the momentum map must be

$$\begin{aligned} \mu(m) &= \int d\mathbf{p} f(\mathbf{x}, \mathbf{p}) + \nabla \cdot \mathbf{Y} \\ &:= \rho + \nabla \cdot \mathbf{Y}, \end{aligned} \quad (3.55)$$

where  $\rho(\mathbf{x}) := \int d\mathbf{p} f(\mathbf{x}, \mathbf{p})$ . Note that, by Eq. (3.54),  $\mu(m) \in \mathfrak{f}^*$  is a density on  $\mathbb{R}^3$ , as desired.

Further observe that  $\mu$  is group equivariant as defined in Eq. (3.36),  $\mu \circ \Phi_\psi = \text{Ad}_{\psi^{-1}}^* \circ \mu$ , where  $\text{Ad}_{\psi^{-1}}^*$  represents the coadjoint action [45] of  $\psi \in \mathcal{F}$  on an element of  $\mathfrak{f}^*$ . In particular, it is clear by inspection of Eq. (3.55) that  $\mu$  is invariant under  $\mathcal{F}$  transformations, and since  $\mathcal{F}$  is abelian, its coadjoint action on  $\mathfrak{f}^*$  is simply the identity map.

## Deriving the conservation law

The momentum map  $\mu$  is defined as in Eqs. (3.51)-(3.52) for any Poisson manifold  $M$  with a canonical group action  $\Phi$ . If it should happen that a Hamiltonian  $H$  is furthermore defined on  $M$  such that  $H$  is invariant under  $\Phi$ , then the momentum map  $\mu$  so-constructed further guarantees a conservation law for the system.

This will now be shown for the Vlasov-Maxwell system. First note that  $\Phi_\psi$  leaves the Hamiltonian invariant,  $\Phi_\psi^* H = H$ . By differentiating this expression with respect to  $\psi$  as in Eq. (3.51), it is seen that, infinitesimally

$$0 = X^\phi(H) = \{\{H, J(\phi)\}\} = -\{\{J(\phi), H\}\} = -\dot{J}(\phi). \quad (3.56)$$

Each linearly independent  $\phi \in \mathfrak{f}$  therefore determines a unique first integral of the system—i.e.,  $J(\phi)$ .

A stronger observation can be made as well. Since  $\dot{J}(\phi) = 0$  holds for arbitrary  $\phi \in \mathfrak{f}$ , the entire momentum map is invariant under the flow of  $H$ , that is

$$\dot{\mu} = \{\{\mu, H\}\} = 0. \quad (3.57)$$

This follows rigorously from the fundamental lemma of variational calculus applied to  $\dot{J}(\phi)$  via Eq. (3.54). As a result, one can apply the definition of Eq. (3.55) to derive

$$0 = \dot{\mu} = \dot{\rho} + \nabla \cdot \dot{\mathbf{Y}}. \quad (3.58)$$

This completes the canonical derivation of the Vlasov-Maxwell local conservation law— $\dot{\mu} = 0$ —in the continuous Hamiltonian formalism. Note that, setting  $\mathbf{Y} = -\mathbf{E}$ , Eq. (3.58) is the time evolution of Gauss's law.

With an additional substitution to Eq. (3.58) from the equations of motion for  $\dot{\mathbf{Y}}$

in Eq. (3.46), this canonical conservation law may be reexpressed in the form

$$0 = \dot{\rho} + \nabla \cdot \mathbf{J}, \quad (3.59)$$

where  $\mathbf{J} := \int f \cdot (\mathbf{p} - \mathbf{A}) d\mathbf{p}$ . Here  $\rho$  and  $\mathbf{J}$  are (scalar and vector) densities over  $\mathbb{R}^3$  and functionals in the sense of Eq. (3.45). This charge conservation law may be immediately checked by substituting the expression for  $\dot{f}$  from Eq. (3.46).

### Reduction of the Vlasov-Maxwell system

Finally, consider the Poisson reduction [57, 58] of the Vlasov-Maxwell system. Consider the particular case  $\alpha = 0$ , and define  $M_0 := \mu^{-1}(0)$ . By Eq. (3.55),  $M_0$  corresponds to the zero level set of  $\mu$ —the submanifold of  $M$  on which  $\rho = -\nabla \cdot \mathbf{Y}$ . Now take equivalence classes of  $M_0$  under the orbit of  $\mathcal{F}$  by defining new phase space coordinates that are invariant under the action of Eq. (3.49), namely

$$\begin{aligned} \bar{f}(\mathbf{x}, \mathbf{v}) &= f(\mathbf{x}, \mathbf{p} = \mathbf{v} + \mathbf{A}) \\ \mathbf{B} &= \nabla \times \mathbf{A} \\ \mathbf{E} &= -\mathbf{Y}. \end{aligned} \quad (3.60)$$

The manifold of equivalence classes  $\tilde{M}_0 := M_0/\mathcal{F}$  is therefore identified with the manifold  $(\bar{f}, \mathbf{B}, \mathbf{E})$  of densities  $\bar{f}$  defined on  $(\mathbf{x}, \mathbf{v})$  space, vector fields  $\mathbf{B}$  that satisfy  $\nabla \cdot \mathbf{B} = 0$ , and vector fields  $\mathbf{E}$  that satisfy  $\bar{\rho} = \nabla \cdot \mathbf{E}$ , where now  $\bar{\rho} := \int \bar{f} d\mathbf{v}$ . (The choice to constrain  $M$  to  $\{m \in M \mid \mu(m) = 0\}$  evidently corresponds to the physical case  $\nabla \cdot \mathbf{E} - \bar{\rho} = 0$ , in which no ‘external’ charges are present in the system.) The reduction map is therefore summarized by

$$\begin{aligned} \pi_{\text{red}} : \quad \mu^{-1}(0) \subset M &\longrightarrow \tilde{M}_0 := \mu^{-1}(0)/\mathcal{F} \\ (f(\mathbf{x}, \mathbf{p}), \mathbf{A}, \mathbf{Y}) &\longmapsto (\bar{f}(\mathbf{x}, \mathbf{v}), \mathbf{B}, \mathbf{E}). \end{aligned} \quad (3.61)$$

As calculated in [59] Sec. 7, the substitution of Eq. (3.60) into the bracket of Eq. (3.39) yields the following reduced Poisson bracket on  $\tilde{M}_0$ :

$$\begin{aligned} \{\{F, G\}\}^{\text{red}}[\bar{f}, \mathbf{B}, \mathbf{E}] &= \int d\mathbf{x}d\mathbf{v} \left[ \bar{f} \left\{ \frac{\delta F}{\delta \bar{f}}, \frac{\delta G}{\delta \bar{f}} \right\}_{\mathbf{x}\mathbf{v}} + \right. \\ &\quad \left. \bar{f}\mathbf{B} \cdot \left( \frac{\partial}{\partial \mathbf{v}} \frac{\delta F}{\delta \bar{f}} \times \frac{\partial}{\partial \mathbf{v}} \frac{\delta G}{\delta \bar{f}} \right) + \left( \frac{\delta F}{\delta \mathbf{E}} \cdot \frac{\partial \bar{f}}{\partial \mathbf{v}} \frac{\delta G}{\delta \bar{f}} - \frac{\delta G}{\delta \mathbf{E}} \cdot \frac{\partial \bar{f}}{\partial \mathbf{v}} \frac{\delta F}{\delta \bar{f}} \right) \right] \\ &\quad + \int d\mathbf{x} \left( \frac{\delta F}{\delta \mathbf{E}} \cdot \nabla \times \frac{\delta G}{\delta \mathbf{B}} - \frac{\delta G}{\delta \mathbf{E}} \cdot \nabla \times \frac{\delta F}{\delta \mathbf{B}} \right). \end{aligned} \quad (3.62)$$

This process of Poisson reduction preserves the  $\dot{\mu} = 0$  conservation law associated with the unreduced Poisson manifold  $M$ . After all, the image of  $\pi_{\text{red}}$  restricts  $M$  to (quotients of) a submanifold  $M_0 \subset M$  on which  $\mu$  is already constant—in particular, level sets of a single value of  $\mu$ . The conservation law of Eq. (3.58) is clearly respected by this reduction, and may simply be reexpressed in the phase space variables of the reduced manifold  $\tilde{M}_0$ , along with its form in Eq. (3.59), i.e.

$$\begin{aligned} 0 = \dot{\mu} &= \dot{\bar{\rho}} - \nabla \cdot \dot{\mathbf{E}} \\ &= \dot{\bar{\rho}} + \nabla \cdot \dot{\mathbf{J}}, \end{aligned} \quad (3.63)$$

where

$$\begin{aligned} \bar{\mu} &= \int d\mathbf{v} \bar{f}(\mathbf{x}, \mathbf{v}) - \nabla \cdot \mathbf{E} \\ &= \bar{\rho} - \nabla \cdot \mathbf{E}, \end{aligned} \quad (3.64)$$

and where  $\bar{\rho} := \int \bar{f} d\mathbf{v}$  and  $\mathbf{J} := \int \bar{f}\mathbf{v} d\mathbf{v}$ .

The reduced bracket of Eq. (3.62) is a well-defined Poisson bracket specifically on the quotient submanifold  $\tilde{M}_0$ . Some of the plasma physics literature [e.g. 15, 67, 68] notes that Eq. (3.62) generally fails to satisfy a Jacobi identity, however, so it is worth elucidating the source of this contrasting point of view.

In particular, the aforementioned literature defines the Vlasov-Maxwell system on

an augmented manifold that includes all unconstrained vector fields  $\mathbf{E}, \mathbf{B} \in \mathbb{R}^3$ :

$$\tilde{M}_0^+ := \tilde{M}_0 \sqcup \{\mathbf{E}, \mathbf{B} \mid \nabla \cdot \mathbf{E} \neq \bar{\rho}, \nabla \cdot \mathbf{B} \neq 0\}. \quad (3.65)$$

When the bracket of Eq. (3.62) is defined on  $\tilde{M}_0^+$  and not on  $\tilde{M}_0$ , it no longer everywhere obeys the Jacobi identity [67, 69]; in particular, the Jacobi identity is satisfied on  $\tilde{M}_0^+$  only when  $\nabla \cdot \mathbf{B} = 0$ . Indeed, the constraint  $\nabla \cdot \mathbf{B} = 0$  appears as an exogenous defect that must be satisfied for  $(\tilde{M}_0^+, \{\{\cdot, \cdot\}\}^{\text{red}})$  to be considered a Poisson manifold. On  $\tilde{M}_0^+$ , the bracket of Eq. (3.62) also acquires additional Casimirs,

$$\begin{aligned} \{\{\cdot, \bar{\rho} - \nabla \cdot \mathbf{E}\}\} &= 0 \\ \{\{\cdot, \nabla \cdot \mathbf{B}\}\} &= 0, \end{aligned} \quad (3.66)$$

in much the same way that a Poisson structure on  $\mathbb{R}^2 = \{(x, y)\}$  acquires a  $z$  Casimir when the system is embedded in  $\mathbb{R}^3$ .

Here, the point of view is adopted that it is more natural to regard the bracket of Eq. (3.62) as a Poisson bracket defined on the submanifold of physical interest— $\tilde{M}_0 = \mu^{-1}(0)/\mathcal{F}$ —rather than a defected bracket defined on the larger manifold including arbitrary vector fields  $\mathbf{E}$  and  $\mathbf{B}$ . In a sense, it is merely a lack of economical notation that leads to the coordinatization  $\tilde{M}_0$  with vector symbols  $\mathbf{E}$  and  $\mathbf{B}$  that are more commonly defined over all of  $\mathbb{R}^3$ . Moreover, it is worth noting that the ‘partially augmented’ manifold  $(\tilde{M}_0 \sqcup \{\mathbf{E} \mid \nabla \cdot \mathbf{E} \neq \bar{\rho}\}, \{\{\cdot, \cdot\}\}^{\text{red}})$  is also a bona fide Poisson manifold.

No matter one’s point of view, it is clear from this discussion that care must be taken in any numerical implementation of the reduced Vlasov-Maxwell bracket to appropriately constrain one’s fields; in general, unconstrained fields  $\mathbf{E}, \mathbf{B} \in \mathbb{R}^3$  are to be avoided.

## 3.2 Lagrangian formalism

Having characterized gauge structure in (continuous) Hamiltonian systems, it will now be studied from quite a different point of view in the Lagrangian formalism. Closely following Olver [53], this section methodically arrives at a concise characterization of variational symmetries in the Lagrangian formalism, from which Noether's theorems are readily shown to follow. The application of this formalism to a vacuum Maxwell action and a Klimontovich-Maxwell action will then be demonstrated.

### 3.2.1 Infinitesimal invariance of a variety

Symmetries of differential equations are helpfully approached by first examining symmetries in a system of algebraic equations defining a variety. To that end, consider a system of  $p \leq r$  functions  $F = (F_1, \dots, F_p)$  on an  $r$ -dimensional smooth manifold  $M$  such that  $F_a \in C^\infty(M) \forall a$ . The *variety* determined by the common zeros of  $F$  is the set  $\mathcal{S}_F = \{m \in M \mid F_a(m) = 0 \forall a\}$ .

A *symmetry group* of  $\mathcal{S}_F$  is a local Lie group  $G$  whose group action  $\Phi$  on  $M$  satisfies  $\Phi_g(\mathcal{S}_F) \subset \mathcal{S}_F \forall g \in G$ . (Here, a *local Lie group* is a set  $G$  that can be imagined as a neighborhood of a Lie group near the identity, which satisfies all Lie group axioms except group closure.) It turns out [53] that, under mild technical assumptions, the question of whether  $G$  is a symmetry group of  $\mathcal{S}_F$  is determined solely by the infinitesimal generators of  $G$  on  $M$ , as defined in Eq. (2.114). Powerfully, a mere ‘first order calculation’ is sufficient to determine the symmetry group of  $\mathcal{S}_F$ .

In particular, assuming  $F$  is everywhere of maximal rank  $p \leq r$  (see Section 2.2.1), a connected local Lie group  $G$  is a symmetry group of  $\mathcal{S}_F \Leftrightarrow$  (if and only if)  $X(F_a) = 0$  wherever  $F = 0, \forall a$  and for every infinitesimal generator  $X$  of  $G$ . The “ $\Rightarrow$ ” direction is immediate since, locally,  $F(\exp(sX)m) = 0$  by necessity  $\forall X \in \mathfrak{g}$  and  $m \in \mathcal{S}_F$ , and  $\frac{d}{ds}F(\exp(sX)m) = X_{\exp(sX)m}(F)$ . The “ $\Leftarrow$ ” direction follows because the maximal

rank condition ensures there are coordinates  $(x^1, \dots, x^r)$  on  $M$  such that  $F(x) = (x^1, \dots, x^\ell)$ . The infinitesimal invariance condition then assures these coordinates are fixed in the flow.

In summary, the symmetry group of  $\mathcal{S}_F$  is determined by the *infinitesimal invariance* of its generators.

### 3.2.2 Jet space

Jet space provides a means of viewing a system of differential equations as if it were a system of algebraic equations. In particular, dependent variables and their derivatives are recast as additional coordinates on jet space, though their interrelatedness requires considerable care. Before describing jet space, it will be useful to establish notation, as follows.

Let

$$\begin{aligned} X &= \{x = (x^1, \dots, x^r)\} = \mathbb{R}^r \\ U &= \{u = (u^1, \dots, u^q)\} = \mathbb{R}^q \end{aligned} \tag{3.67}$$

be independent and dependent variables, respectively, of a system  $\mathcal{S}$  of differential equations with solutions of the form  $u = f(x)$ , such that  $f : X \rightarrow U$ . A  $(k \geq 0)$ -*order multi-index*  $J$  is defined by  $J = (j_1, \dots, j_k)$ , where  $1 \leq j_i \leq r$ .  $\#J$  denotes the order (i.e., length) of the multi-index  $J$ , where any repetitions of indices are to be double-counted. Accordingly,  $u_{,J}$  represents a partial derivative taken with respect to  $(x^{j_1}, \dots, x^{j_k})$ .  $u_{,ii} = \partial^2 u / \partial x^i \partial x^i$  has  $\#J = 2$ , for example.  $D_i$  will denote a *total derivative* in the usual sense, i.e.

$$D_i P := \frac{\partial P}{\partial x^i} + \sum_{\ell=1}^q \sum_{\#J \geq 0} u_{,Ji}^\ell \frac{\partial P}{\partial u_{,J}^\ell} \tag{3.68}$$

and  $D_J = D_{j_1} \cdots D_{j_k}$ . The operator  $(-D)_J$  denotes a total derivative with negative

signs included for each index, for example:

$$(-D)_{xyz}u = (-D_x)(-D_y)(-D_z)u = -\frac{\partial^3 u}{\partial x \partial y \partial z} = -u_{xyz}. \quad (3.69)$$

A symmetry group  $G$  of  $\mathcal{S}$  must act on  $X \times U$  in such a way that solutions  $u = f(x)$  of  $\mathcal{S}$  are transformed into other solutions  $\tilde{u} = \tilde{f}(\tilde{x})$  of  $\mathcal{S}$ .<sup>(\*)</sup> However, when  $x$  or  $u$  is transformed, the derivatives  $u_{,j}$  transform as well. To use the infinitesimal invariance criterion of the last section, therefore, care must be taken to ensure that transformations are properly calculated for higher order terms in a system of differential equations.

To facilitate such a calculation, the  $n^{\text{th}}$ -order jet space of  $X \times U$  is defined as

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(\*) Note, this condition states that the function  $f$  of  $x$  will be (implicitly) transformed into a new function  $\tilde{f}$  of  $\tilde{x}$ . The relevant question is whether this new function satisfies a *fixed* system of differential equations.

As a simple example adapted from Olver [53], take  $X \times U = \mathbb{R}^2$  and consider the ODE  $u_{,xx} = 0$ . Solutions are clearly given by any linear function  $u = f(x) = ax + b$ . An  $SO(2)$  rotation of the plane by  $\theta$  defines the transformation

$$\begin{pmatrix} \tilde{x} \\ \tilde{u} \end{pmatrix} = \begin{pmatrix} \theta \cdot x \\ \theta \cdot u \end{pmatrix} = \begin{pmatrix} x \cos \theta - u \sin \theta \\ x \sin \theta + u \cos \theta \end{pmatrix}. \quad (3.70)$$

To solve for  $\tilde{f}(\tilde{x})$ , one can substitute  $u = f(x) = ax + b$  and solve for  $x(\tilde{x})$ . In particular,

$$\tilde{x} = x \cos \theta - (ax + b) \sin \theta \Rightarrow x = \frac{\tilde{x} + b \sin \theta}{\cos \theta - a \sin \theta}. \quad (3.71)$$

Then, substituting for  $x$  and  $u$  in  $\tilde{u}$ ,

$$\begin{aligned} \tilde{u} &= \frac{\tilde{x} + b \sin \theta}{\cos \theta - a \sin \theta} \sin \theta + \left( a \frac{\tilde{x} + b \sin \theta}{\cos \theta - a \sin \theta} + b \right) \cos \theta \\ &= \left( \frac{\sin \theta + a \cos \theta}{\cos \theta - a \sin \theta} \right) \tilde{x} + \left( \frac{b}{\cos \theta - a \sin \theta} \right) \\ &= A\tilde{x} + B. \end{aligned} \quad (3.72)$$

Thus,  $\tilde{f}(\tilde{x}) = A\tilde{x} + B$  is a different linear function with new constants; (as expected, rotations of the plane preserve lines). Since  $\tilde{u} = \tilde{f}(\tilde{x})$  is still a solution of the ODE  $\tilde{u}_{,\tilde{x}\tilde{x}} = 0$ ,  $SO(2)$  is a symmetry group of the ODE.

Here, the system of differential equations is regarded as *fixed* in that it can be treated as an algebraic function of jet space coordinates (see Eq. (3.73)). Even as those coordinates  $[u] = (x, u, u_{,x}, u_{,xx}, \dots)$  are transformed into  $[\tilde{u}] = (\tilde{x}, \tilde{u}, \tilde{u}_{,\tilde{x}}, \tilde{u}_{,\tilde{x}\tilde{x}}, \dots)$ , should the transformed coordinates  $[\tilde{u}]$  continue to satisfy the same algebraic equation, the transformation is regarded as a symmetry of the system.

$X \times U^{(n)} = X \times U \times U^1 \times \cdots \times U^n$ , whose coordinates are given by  $x$ ,  $u$ , and all derivatives of  $u$  up to order  $n$ , respectively. Given the simplest case  $X \times U = \mathbb{R}^2$ , for example,  $X \times U^{(1)}$  is a three-dimensional space coordinatized by  $(x, u^{(1)}) = (x, u, u_x)$ . Hereafter, a shorthand  $[u]$  will be used to denote

$$[u] = (x, u^{(n)}). \quad (3.73)$$

It is now clear that a system of  $n^{\text{th}}$  order differential equations is a variety in  $X \times U^{(n)}$ , upon which the infinitesimal invariance methods of the previous section can be applied. In particular, the system of  $n^{\text{th}}$  order differential equations

$$\Delta_a[u] = 0 \quad a = 1, \dots, p \quad (3.74)$$

is defined by the variety  $\mathcal{S}_\Delta = \{(x, u^{(n)}) \mid \Delta_a[u] = 0 \forall a\}$  in  $n^{\text{th}}$ -order jet space. In this setting,  $\Delta_a[u]$  can conveniently be viewed as an algebraic function of the inputs, rather than as a differential operator. The cost for this convenience, however, is the need to consider the interrelatedness between jet space coordinates when performing an infinitesimal transformation, an effort that can be achieved by *prolongation*—which shall now be described.

### 3.2.3 Prolongation and infinitesimal invariance of differential equations

In particular, given a function  $u = f(x)$ , (equivalently, a mapping  $f : X \rightarrow U$ ), another mapping  $\text{pr}^{(n)}f : X \rightarrow U^{(n)}$  called the *prolongation of  $f$*  is uniquely induced with an image in jet space, defined by  $u_{,J}^\ell = \partial_J f^\ell(x)$ . For the case  $X \times U = \mathbb{R}^2$ , for example,  $\text{pr}^{(2)}f = (f, \partial_x f, \partial_x^2 f)$ .

Extending this result, given an arbitrary vector field  $Y \in \mathfrak{X}(X \times U)$  of the form

$$Y = Q^\ell[u] \frac{\partial}{\partial u^\ell}, \quad (3.75)$$

—whose coefficients  $Q^\ell[u]$  may depend upon higher order jet space coordinates as in Eq. (3.73)—the prolongation of  $Y$  on  $X \times U^{(n)}$ , denoted  $\text{pr}^{(n)}Y \in \mathfrak{X}(X \times U^{(n)})$ , is defined by

$$\text{pr}^{(n)}Y = \sum_{\#J \geq 0} \left( D_J Q^\ell[u] \right) \frac{\partial}{\partial u_J^\ell}. \quad (3.76)$$

Here, Einstein summation convention is assumed for the index  $\ell$  in Eqs.(3.75)-(3.76), and terms are kept up to  $n^{\text{th}}$  order on jet space. The  $q$ -tuple  $Q[u] = (Q^1, \dots, Q^q)$  is called the *characteristic* of  $Y$ .

$\text{pr}^{(n)}Y$  thereby generates transformations of  $X \times U^{(n)}$  that are self-consistent with those generated by  $Y$  on  $X \times U$ . Therefore, the same classification of a symmetry group described in Section 3.2.1 for algebraic systems applies; given a system  $\{\Delta_a\}$  of  $n^{\text{th}}$  order differential equations defined over  $X \times U$  as in Eq. (3.74), and given a local group  $G$  of transformations on  $X \times U$ , if  $\text{pr}^{(n)}Y(\Delta_a) = 0$  for all infinitesimal generators  $Y$  of  $G$  and for all  $a$ , then  $G$  is a symmetry group of  $\{\Delta_a\}$ .

### 3.2.4 Lagrangian dynamics

Hamilton’s principle, which posits that physical systems evolve according to variational principles, is among the most crucial convictions of physics. The Lagrangian of a system offers—in a single object—a recipe for its dynamics and an accessible accounting of its symmetries.

A physical system is conveniently described on jet space  $X \times U^{(n)}$  via the *action*

functional

$$\mathcal{S}[u] = \int_{\Omega} \mathcal{L}[u] dx \quad (3.77)$$

where  $\Omega \subset X$  is assumed open and connected with smooth boundary  $\partial\Omega$ . Hamilton's principle holds that evolutions of the system are extremals of  $\mathcal{S}[u]$ , such that its dependent variables evolve as  $u = f(x)$ , where  $f \in C^\infty(\Omega, \mathbb{R}^q)$  satisfies

$$\left. \frac{d}{ds} \right|_{s=0} \mathcal{S}[f + s\eta] = 0 \quad (3.78)$$

$\forall \eta \in C^\infty(\overset{\circ}{\Omega}, \mathbb{R}^q)$ . (Here,  $\overset{\circ}{\Omega}$  signifies the restriction of  $\eta$  to smooth functions with compact (closed and bounded) support in the interior of  $\Omega$ , ensuring that  $f + s\eta$  satisfies the same boundary conditions as may be required of  $f$ .)

The differentiation of Eq. (3.78) is facilitated by the *variational derivative of  $\mathcal{S}$* , defined as the unique  $q$ -tuple  $\delta\mathcal{S}[u] = \left( \frac{\delta\mathcal{S}[u]}{\delta u^1}, \dots, \frac{\delta\mathcal{S}[u]}{\delta u^q} \right)$  such that

$$\left. \frac{d}{ds} \right|_{s=0} \mathcal{S}[f + s\eta] = \int_{\Omega} \delta\mathcal{S}[f(x)] \cdot \eta(x) dx \quad (3.79)$$

$\forall f \in C^\infty(\Omega, \mathbb{R}^q)$  and  $\eta \in C^\infty(\overset{\circ}{\Omega}, \mathbb{R}^q)$ . By the fundamental lemma of the calculus of variations, when  $u = f(x)$  is an extremal of  $\mathcal{S}[u]$  (defined as in Eq. (3.78)), it clearly follows that  $\delta\mathcal{S}[f(x)] = 0$ .

$\delta\mathcal{S}[u]$  can be explicitly calculated by the following derivation:

$$\begin{aligned}
\left. \frac{d}{ds} \right|_{s=0} \mathcal{S}[f + s\eta] &= \int_{\Omega} \left. \frac{d}{ds} \right|_{s=0} \mathcal{L}[f(x) + s\eta(x)] dx \\
&= \int_{\Omega} \sum_{\#J \geq 0} \frac{\partial \mathcal{L}[f(x)]}{\partial u_{,J}^{\ell}} \cdot \partial_J \eta^{\ell} dx \\
&= \int_{\Omega} \sum_{\#J \geq 0} (-D)_J \frac{\partial \mathcal{L}[f(x)]}{\partial u_{,J}^{\ell}} \cdot \eta^{\ell}(x) dx \\
&= \int_{\Omega} E_{\ell}(\mathcal{L}[f(x)]) \cdot \eta^{\ell}(x) dx
\end{aligned} \tag{3.80}$$

where the first line follows from the Leibniz integral rule, and the third line follows from integration by parts. In the final line, the *Euler operator* has been introduced, explicitly defined by

$$E_{\ell} = \sum_{\#J \geq 0} (-D)_J \frac{\partial}{\partial u_{,J}^{\ell}}. \quad \ell \in \{1, \dots, q\} \tag{3.81}$$

These determine the extremals of  $\mathcal{S}[u]$ , and therefore the dynamical *Euler-Lagrange equations* of the physical system defined by  $\mathcal{S}[u]$ , namely,

$$E_{\ell}(\mathcal{L}) = 0 \quad \ell \in \{1, \dots, q\}. \tag{3.82}$$

It is well known that adding a divergence term to a Lagrangian leaves its equations of motion invariant, that is,  $E_{\ell}(\mathcal{L} + \text{Div}A) = E_{\ell}(\mathcal{L})$ , where  $\text{Div}A = D_i A^i$  for any  $r$ -tuple  $A[u] = (A^1[u], \dots, A^r[u])$  of smooth functions on jet space (that is,  $A^i \in C^{\infty}(X \times U^{(n)}) \forall i \in \{1, \dots, r = \mathbf{dim}X\}$ ). This follows from an important property of the Euler operator, namely, that it annihilates divergences

$$E_{\ell} \circ \text{Div} = 0, \tag{3.83}$$

a fact that can be directly checked using Eqs. (3.68) and (3.81).

### 3.2.5 Noether's theorems (N1T and N2T) in Lagrangian systems

Since divergences vanish under the Euler operator, the equations of motion of a variational system  $\mathcal{S}[u] = \int_{\Omega} \mathcal{L}[u] dx$  are invariant under a transformation of the form

$$\tilde{\mathcal{L}}[\tilde{u}] = \mathcal{L}[u] + \text{Div}A[u] \quad (3.84)$$

$\forall A[u]$  an arbitrary  $r$ -tuple.

Accordingly, using the prolongation formula of Eq. (3.76), a *variational symmetry* is defined as one which meets the the following infinitesimal criterion when applied to the Lagrangian defined by  $\mathcal{L}[u]$ :

$$\text{pr}^{(n)}Y(\mathcal{L}) = \text{Div}A \quad (3.85)$$

for any  $A[u] = (A^1[u], \dots, A^r[u])$ .

Letting the  $q$ -tuple  $Q[u] = (Q^1, \dots, Q^q)$  denote the characteristic of  $Y$  as in Eq. (3.75), a particularly enlightening form of the symmetry condition Eq. (3.85) follows from substituting the prolongation formula of Eq. (3.76), namely:

$$\begin{aligned} 0 &= \sum_{\#J \geq 0} \left( D_J Q^\ell[u] \right) \frac{\partial \mathcal{L}}{\partial u^\ell_{,J}} - \text{Div}A \\ &= \sum_{\#J \geq 0} Q^\ell[u] (-D_J) \frac{\partial \mathcal{L}}{\partial u^\ell_{,J}} + \text{Div}A' - \text{Div}A \\ &= Q^\ell[u] E_\ell(\mathcal{L}) - \text{Div}B \end{aligned} \quad (3.86)$$

where the second line integrates by parts, noting that any boundary terms that arise can be collected into a divergence  $\text{Div}A'$ . Thus, a condition equivalent to Eq. (3.85) for establishing a variational symmetry of a Lagrangian system is the existence of

characteristics  $Q[u] = (Q^1[u], \dots, Q^q[u])$  such that

$$Q^\ell[u]E_\ell(\mathcal{L}) = \text{Div}B \quad (3.87)$$

for any  $r$ -tuple  $B[u]$ . As is now demonstrated Noether's two theorems readily follow from this criterion for a variational symmetry.

From the symmetry criterion of Eq. (3.87), it readily follows that when the Lagrangian system  $\mathcal{S}[u] = \int \mathcal{L}[u]dx$  evolves on-shell, that is when  $E_\ell(\mathcal{L}) = 0 \forall \ell$ , a corresponding conservation law holds, namely

$$\text{Div}B = 0. \quad (3.88)$$

This is the essential content of *Noether's first theorem (N1T)*, which establishes that each variational symmetry of  $\mathcal{L}$  gives rise to a corresponding conservation law.

On the other hand, suppose that a Lagrangian system admits a variational symmetry whose characteristics  $Q[u; \boldsymbol{\lambda}(x)]$  depend freely upon an arbitrary, unconstrained function of spacetime— $\boldsymbol{\lambda}(x)$ —and its derivatives. (Such a variational symmetry will be referred to as a *local* variational symmetry.) Then, treating  $\boldsymbol{\lambda}(x)$  as if it were a dynamical variable, its Euler operator  $E_\lambda$  can be defined according to Eq. (3.81), and applied to both sides of Eq. (3.87). Since Euler operators always annihilate divergences, as noted in Eq. (3.83),  $E_\lambda$  zeros  $\text{Div}B$  on the right hand side, resulting in the expression

$$E_\lambda \left[ Q^\ell[u; \boldsymbol{\lambda}]E_\ell(\mathcal{L}) \right] = 0. \quad (3.89)$$

Eq. (3.89) is a relation that holds identically—even when  $E_\ell(\mathcal{L}) \neq 0 \forall \ell$  and the system is off-shell. When  $Q[u; \boldsymbol{\lambda}]$  is linear in  $\boldsymbol{\lambda}$ , it is clear that  $\boldsymbol{\lambda}$  vanishes from

Eq. (3.89), leaving a differential identity of the Euler-Lagrange equations of the form

$$\mathcal{D}^\ell \mathbf{E}_\ell(\mathcal{L}) = 0 \quad (3.90)$$

for some  $q$ -tuple of differential operators  $(\mathcal{D}^1, \dots, \mathcal{D}^q)$ . This is the essential content of *Noether's second theorem (N2T)*, which establishes that each local variational symmetry of  $\mathcal{L}$  gives rise to a corresponding differential identity of the Euler-Lagrange equations.

Several notes about this result are in order. First, it should be specified that  $\{\mathcal{D}^\ell\}$  are specified by finite sums of the form  $\mathcal{D}^\ell = \sum_J P^{\ell,J}[u] \mathbf{D}_J$  for smooth functions  $P^{\ell,J}[u] \in C^\infty(X \times U^{(n)})$ . Second, when  $Q[u; \boldsymbol{\lambda}]$  is nonlinear in  $\boldsymbol{\lambda}$ , Eq. (3.89) is not necessarily independent of  $\boldsymbol{\lambda}$ . In this case, the N2T identity independent of  $\boldsymbol{\lambda}$  can be found by replacing  $Q^\ell[u; \boldsymbol{\lambda}]$  in Eq. (3.89) with its (sufficiently high order) *Fréchet derivative with respect to  $\boldsymbol{\lambda}$* , e.g.  $\mathbf{D}_{Q^\ell}(\mathbf{h}) = \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} Q^\ell[u; \boldsymbol{\lambda} + \epsilon \mathbf{h}]$ . (See [53], Definition 5.24.) Lastly, note that the N2T relationship established between a local variational symmetry and a differential identity is *if and only if*. That is, not only can Eq. (3.90) be derived from Eq. (3.87), but starting with Eq. (3.90), a local variational symmetry can be found by integrating  $\boldsymbol{\lambda}(x) \cdot \mathcal{D}^\ell \mathbf{E}_\ell(\mathcal{L}) = 0$  by parts (for arbitrary  $\boldsymbol{\lambda}$ ) to derive an expression of the form Eq. (3.87).

### 3.2.6 Example: N2T for the vacuum Maxwell action

To make the preceding formalism more concrete, consider the following example that calculates a differential identity from the vacuum Maxwell action,

$$S = \int d^4x \mathcal{L} = -\frac{1}{4} \int d^4x F_{\mu\nu} F^{\mu\nu}, \quad (3.91)$$

where  $F_{\mu\nu} \equiv \partial_\mu A_\nu - \partial_\nu A_\mu$ . This action yields the familiar equations of motion

$$0 = \mathbf{E}_{A_\sigma}(\mathcal{L}) = \left[ \frac{\partial}{\partial A_\sigma} - \mathbf{D}_\tau \frac{\partial}{\partial(\partial_\tau A_\sigma)} + \dots \right] \mathcal{L} = \partial_\tau F^{\tau\sigma}. \quad (3.92)$$

Note that, for arbitrary smooth  $\lambda(x)$ ,  $\mathcal{L}$  is invariant under the local gauge transformation  $A_\mu(x) \rightarrow A_\mu(x) - \partial_\mu \lambda(x)$ . In particular, the infinitesimal generator of this gauge transformation is given by the following vector field with characteristics given by the 4-tuple  $Q^{A_\mu}[\lambda] = -\partial_\mu \lambda$ :

$$\mathbf{v}_\lambda = -(\partial_\mu \lambda) \partial_{A_\mu} \quad \Rightarrow \quad \text{pr}^{(1)} \mathbf{v}_\lambda = -(\partial_\mu \lambda) \partial_{A_\mu} - (\partial_\nu \partial_\mu \lambda) \partial_{(\partial_\nu A_\mu)}. \quad (3.93)$$

Here, as above, the Einstein summation convention over Greek indices is assumed.

To check that this vector field generates the desired transformation, note via Eq. (2.71) that the flow generated by  $\mathbf{v}_\lambda$  on the product manifold  $X \times \{A_\mu\}$  transforms  $A_\mu$  appropriately:

$$\begin{aligned} \exp[\mathbf{v}_\lambda](x^\rho, A_\sigma) &= \left[ \mathbb{1} + \mathbf{v}_\lambda + \frac{1}{2!} \mathbf{v}_\lambda^2 + \dots \right] (x^\rho, A_\sigma) \\ &= \left[ \mathbb{1} - (\partial_\mu \lambda) \partial_{A_\mu} + \frac{1}{2!} (\partial_\mu \lambda)^2 \partial_{A_\mu}^2 + \dots \right] (x^\rho, A_\sigma) \\ &= (x^\rho, A_\sigma - \partial_\sigma \lambda). \end{aligned} \quad (3.94)$$

Moreover, the invariance criterion of Eq. (3.85) is readily seen—namely,  $\text{pr}^{(1)} \mathbf{v}_\lambda(\mathcal{L}) = 0$ .

Given the equations of motion in Eq. (3.92) and the symmetry characteristics in Eq. (3.93),  $\mathbf{E}_{u^\alpha}(\mathcal{L})$  and  $Q^\alpha[\lambda]$  can simply be plugged into Eq. (3.89) to derive this system's N2T differential identity:

$$\begin{aligned} 0 &= \mathbf{E}_\lambda \left[ -(\partial_\sigma \lambda) \partial_\tau F^{\tau\sigma} \right] \\ &= \partial_\sigma \partial_\tau F^{\tau\sigma}. \end{aligned} \quad (3.95)$$

As expected, because of the linearity of  $\lambda(x)$  in  $Q^{A\mu}[\lambda]$ ,  $\lambda(x)$  vanishes from Eq. (3.95).

Eq. (3.95) is the resultant N2T differential identity. Due to the antisymmetry of  $F^{\mu\nu}$ , this identity conveys the appropriate sense that N2T produces off-shell identities independent of a system's dynamics, and it may appear, at first, rather uninformative.

In fact, Eq. (3.95) reveals an important attribute of Maxwell's equations. In particular, Eq. (3.92) would appear to be four equations  $\partial_\tau F^{\tau\sigma} = 0$  in four unknowns  $A_\mu$ , and one might therefore suspect Maxwell's equations to be completely determined. However, N2T demonstrates that Eq. (3.92) represents only three independent equations, since their particular combination in the identity of Eq. (3.95) is satisfied automatically. (This is consistent with the fact that gauge-fixing Maxwell's equations requires only a single scalar condition, such as  $\phi = 0$ , to determine them.) The N2T differential identity automatically detects this important consequence of gauge symmetry.

### 3.2.7 Example: N2T for the Klimontovich-Maxwell action

Another example of the preceding N2T procedure is demonstrated to systematically derive a charge conservation law for the Klimontovich-Maxwell system,<sup>(\*)</sup> described by the following action:

$$S = \int d^4x \mathcal{L}[\phi, \mathbf{A}, \mathbf{X}_i] = \int d^4x \left[ \frac{1}{2}(\nabla\phi + \partial_t\mathbf{A})^2 - \frac{1}{2}(\nabla \times \mathbf{A})^2 + \sum_{j=1}^N \delta_j \cdot \left( \frac{1}{2}m_j\dot{\mathbf{X}}_j^2 - q_j\phi + q_j\mathbf{A} \cdot \dot{\mathbf{X}}_j \right) \right]. \quad (3.97)$$

---

<sup>(\*)</sup> This system specializes a Vlasov-Maxwell system to the following distribution function defined by  $N$  point particles

$$f(t, \mathbf{x}, \mathbf{v}) = \sum_{j=1}^N \delta^{(3)}(\mathbf{x} - \mathbf{X}_j(t))\delta^{(3)}(\mathbf{v} - \dot{\mathbf{X}}_j(t)). \quad (3.96)$$

Here,  $\mathbf{A} = \mathbf{A}(t, \mathbf{x})$  is the vector potential,  $\phi = \phi(t, \mathbf{x})$  is the electric potential,  $\mathbf{X}_i = \mathbf{X}_i(t)$  are particle positions and particle mass and charge are denoted by  $m_i$  and  $q_i$ , respectively. The following shorthand has also been used for the delta function:

$$\delta_j := \delta^{(3)}(\mathbf{x} - \mathbf{X}_j(t)). \quad (3.98)$$

Applying Euler operators to derive the Euler-Lagrange equations of each field yields

$$\begin{aligned} \mathbf{E}_\phi(\mathcal{L}) &= \nabla \cdot \mathbf{E} - \rho \\ \mathbf{E}_\mathbf{A}(\mathcal{L}) &= \partial_t \mathbf{E} - \nabla \times \mathbf{B} + \mathbf{J} \\ \mathbf{E}_{\mathbf{X}_i}(\mathcal{L}) &= \delta_i \cdot \left[ -m_i \ddot{\mathbf{X}}_i + q_i (\mathbf{E} + \dot{\mathbf{X}}_i \times \mathbf{B}) \right] \end{aligned} \quad (3.99)$$

where the distributional derivative

$$\int f(\eta) \delta'(\eta) d\eta = - \int f'(\eta) \delta(\eta) d\eta \quad (3.100)$$

with  $\eta \in \{t, \mathbf{x}\}$  has been applied, and where

$$\begin{aligned} \mathbf{E}(t, \mathbf{x}) &:= -\nabla \phi(t, \mathbf{x}) - \partial_t \mathbf{A}(t, \mathbf{x}) \\ \mathbf{B}(t, \mathbf{x}) &:= \nabla \times \mathbf{A}(t, \mathbf{x}) \\ \rho(t, \mathbf{x}) &:= \sum_{j=1}^N q_j \delta_j \\ \mathbf{J}(t, \mathbf{x}) &:= \sum_{j=1}^N q_j \dot{\mathbf{X}}_j(t) \delta_j. \end{aligned} \quad (3.101)$$

Now consider transforming the action of Eq. (3.97) under the following gauge

transformation:

$$\begin{aligned}\phi &\rightarrow \phi' = \phi + \partial_t \lambda \\ \mathbf{A} &\rightarrow \mathbf{A}' = \mathbf{A} - \nabla \lambda.\end{aligned}\tag{3.102}$$

The vector field generating this transformation—equivalent to Eq. (3.93)—is given by

$$\mathbf{v}_\lambda = \sum_\alpha Q^\alpha[\lambda] \partial_{u^\alpha} = (\partial_t \lambda) \partial_\phi - (\nabla \lambda) \cdot \partial_{\mathbf{A}}\tag{3.103}$$

for an arbitrary smooth function  $\lambda(x)$ , and it is seen that

$$\text{pr}^{(1)} \mathbf{v}_\lambda(\mathcal{L}) = \partial_\mu \gamma^\mu \quad \text{where} \quad \gamma^\mu = - \sum_j q_j \delta_j \lambda \cdot (1, \dot{\mathbf{X}}_j).\tag{3.104}$$

In particular, the electromagnetic terms of the Lagrangian are invariant, while the coupled particle terms pick up a divergence that vanishes under the Euler operator. Therefore, the invariance criterion of Eq. (3.85) is satisfied.

Thus, given equations of motion in Eq. (3.99) and characteristics of the gauge symmetry in Eq. (3.103)—that is,

$$\begin{aligned}\sum_\alpha Q^\alpha[\lambda] \mathbf{E}_{u^\alpha}(\mathcal{L}) &= Q^\phi[\lambda] \cdot \mathbf{E}_\phi(\mathcal{L}) + Q^{\mathbf{A}}[\lambda] \cdot \mathbf{E}_{\mathbf{A}}(\mathcal{L}) \\ &= (\partial_t \lambda) [\nabla \cdot \mathbf{E} - \rho] - \nabla \lambda \cdot [\partial_t \mathbf{E} - \nabla \times \mathbf{B} + \mathbf{J}]\end{aligned}\tag{3.105}$$

—the N2T differential identity can be computed from Eq. (3.89), such that

$$\begin{aligned}0 &= \mathbb{E}_\lambda \left[ \sum_\alpha Q^\alpha[\lambda] \mathbf{E}_{u^\alpha}(\mathcal{L}) \right] \\ &= -\partial_t [\nabla \cdot \mathbf{E} - \rho] + \nabla \cdot [\partial_t \mathbf{E} - \nabla \times \mathbf{B} + \mathbf{J}] \\ &= \partial_t \rho + \nabla \cdot \mathbf{J}.\end{aligned}\tag{3.106}$$

In the final line, the equality of mixed partials and the vanishing divergence of the curl are used.

The N2T differential identity arising from the Klimontovich-Maxwell Lagrangian's local gauge symmetry evidently discovers the charge conservation law itself. By construction, this conservation law must hold off-shell and identically; in particular, Eq. (3.106) does not require the equations of motion in order to hold true. It is a trivial conservation law—also referred to as a ‘strong’ or ‘improper’ conservation law [70]—an often-overlooked fact that is immediately verified upon examining the definitions of  $\rho$  and  $\mathbf{J}$  in Eq. (3.101).

# 4

## Elements of Structure-Preserving Algorithms

In this chapter, relevant principles and tools of structure-preserving algorithms are reviewed. While much of this chapter recapitulates known results, the first original contributions of the thesis appear in this chapter, namely the classification of gauge-compatible splitting methods.

First, two discretizations methods shall be briefly reviewed—discrete exterior calculus [32, 33] and finite element exterior calculus [34, 35]. The discretizations employed in structure-preserving algorithms play an important role in the preservation of gauge structure. Indeed, a careful examination of gauge structure reveals that a successful discretization must preserve topological features of the continuous manifold.

### 4.1 Discrete Exterior Calculus (DEC)

The essential constituents of DEC are  $k$ -simplices  $\sigma^k = [v_0, \dots, v_k]$ , defined as the convex span of  $(k + 1)$  geometrically independent points  $v_i$  in  $\mathbb{R}^{n \geq k}$ . Even (odd) permutations of the vertices of  $\sigma^k$  are said to be positively (negatively) oriented. Any

subset of  $\{v_0, \dots, v_k\}$  defines a *face* of  $\sigma^k$ . The *boundary* of  $\sigma^k$ , denoted  $\partial\sigma^k$  is defined by

$$\partial\sigma^k = \sum_{i=0}^k (-1)^i [v_0, \dots, \hat{v}_i, \dots, v_k], \quad (4.1)$$

where the hat denotes omission of  $v_i$  in the  $i^{\text{th}}$  term of the sum.

A *simplicial complex*  $K$  is a collection of simplices obeying just two properties:

- every face of a simplex of  $K$  is in  $K$ ; and
- the intersection of two simplices of  $K$  is a face of them both.

Differential forms are represented in DEC using elements of algebraic topology (accessible introductions can be found in [71, 72]). Oriented  $k$ -simplices are taken as basis elements of the free abelian group of  $k$ -chains, denoted  $C_k(K, \mathbb{R})$ . More concretely, a  $k$ -chain is nothing more than a formal linear combination of oriented  $k$ -simplices with coefficients over  $\mathbb{R}$ . A discrete differential form, then, or a  $k$ -cochain, is defined as a linear map from the set of  $k$ -chains to  $\mathbb{R}$ .

A  $k$ -cochain can be usefully described by the dual basis to  $C_k(K, \mathbb{R})$ . A discrete 0-form  $\alpha$ , for example, can be defined by its coefficients at each vertex, and a discrete 1-form  $\beta$  by its coefficients on each edge:

$$\begin{aligned} \alpha &= \alpha_i \Delta^i \\ \beta &= \beta_{ij} \Delta^{ij}. \end{aligned} \quad (4.2)$$

Here,  $\Delta^i$  denotes the 0-cochain that evaluates to 1 on the vertex  $[v_i]$  and 0 on other vertices. Similarly,  $\Delta^{ij}$  denotes the 1-cochain that evaluates to 1 on the edge  $[v_i v_j]$  and 0 elsewhere.

The exterior derivative in DEC is implemented as a formal adjoint to the boundary

operator  $\partial$ . This adjoint is defined by the coboundary operator  $\delta$ , satisfying

$$\langle \delta \alpha^k, c_{k+1} \rangle = \langle \alpha^k, \partial c_{k+1} \rangle \quad (4.3)$$

for any  $(k+1)$ -chain  $c_{k+1}$  and  $k$ -cochain  $\alpha^k$ . Here,  $\langle \cdot, \cdot \rangle$  denotes the bilinear pairing of cochains and chains.

Denoting the set of labels for all vertices in  $K$  by  $\{v\}$ , those for edges by  $\{e\}$ , and those for faces by  $\{f\}$ ,  $\delta$  may therefore be defined [73, 74] by a matrix multiplication in the cochain basis. For a 1-form  $\beta$ , for example:

$$\delta \beta = \delta (\beta_e \Delta^e) = \beta_e \delta \Delta^e = \beta_e W_f^e \Delta^f \quad (4.4)$$

where the matrix entry  $W_f^e$  stores the weight— $\{\pm 1, 0\}$ —of the 1-cochain  $\Delta^e$  in the 2-cochain  $\Delta^f$ . (As its adjoint, the boundary operator on chains— $\partial$ —can likewise be computed from  $W_e^f = (W_f^e)^T$ .) Einstein summation convention is adopted in Eq. (4.4) for the labels of corresponding simplices.

Since DEC is defined with elements of algebraic topology, its implementation of the Hodge star necessitates the use of *dual cells* that are distinct from the *primal cells*, that is, from the simplices that define  $K$ . DEC implements this construction via a circumcentric subdivision of primal cells. The dual-form  $\star \alpha$  is then defined on a dual chain  $\star \sigma$  as follows:

$$\langle \star \alpha, \star \sigma \rangle = \epsilon(\sigma) \frac{|\star \sigma|}{|\sigma|} \langle \alpha, \sigma \rangle, \quad (4.5)$$

where  $\epsilon(\sigma)$  appropriately reflects the signature of the metric and its relation to the cell

$\sigma$ . In a Euclidean space,  $\epsilon(\sigma) = 1 \forall \sigma$ , but in a 4-dimensional Lorentzian spacetime,

$$\epsilon(\sigma) = \begin{cases} +1 & \text{if } \sigma \text{ is entirely spacelike} \\ -1 & \text{otherwise.} \end{cases} \quad (4.6)$$

Here,  $|\sigma^k|$  denotes the  $k$ -volume of the  $k$ -dimensional  $\sigma^k$  (where  $|\sigma^0| = 1$  for a single vertex).

Interpolations of DEC forms can be facilitated using Whitney forms [36], which will be elaborated upon in the discussion of finite element exterior calculus. In particular, Whitney forms enjoy a natural compatibility between their interpolations of the discrete coboundary operator and the continuous exterior derivative of their interpolations, i.e.

$$(\delta\alpha)_{\text{interp}} = d(\alpha)_{\text{interp}}, \quad (4.7)$$

so that the discrete operator  $\delta$  behaves as an exact discretization of  $d$  on the discrete form  $\alpha$ . Indeed, the relationship between these operators is so strong that the notation  $d$  will henceforth be employed for  $\delta$ .

## 4.2 Finite Element Exterior Calculus (FEEC)

Relevant aspects of finite element exterior calculus (FEEC) [34, 35] are now described. FEEC hews more closely to the description of differential forms in continuous space than its counterpart DEC. In particular, in FEEC, one does not imagine ‘interpolating’ forms defined on  $k$ -chains of a simplex. Rather, FEEC simply treats differential forms in continuous space, which just ‘happen to be’ piecewise continuous, with higher order discontinuities at interfaces and edges. Although there is a direct mapping between low order implementations of FEEC and DEC, the method of

FEEC is more generalizable and robust. As one example of this, the implementation of the Hodge star, which has several interpretations in DEC (only one of which was described in the last section), is uniquely determined in FEEC.

To approximate differential forms on a smooth manifold  $\Omega$  by finite elements, one begins with the de Rham complex of differential forms on  $\Omega$ ,  $0 \xrightarrow{d} \Lambda^0(\Omega) \xrightarrow{d} \dots \xrightarrow{d} \Lambda^n(\Omega) \xrightarrow{d} 0$ . Each space of continuous  $p$ -forms may be restricted to a well-behaved subspace  $L^2\Lambda^p(\Omega) \subset \Lambda^p(\Omega)$  of  $p$ -forms that yield  $L^2$ -integrable functions when evaluated on arbitrary smooth vector fields on  $\Omega$ . That is, denoting  $\omega(\mathbf{X}) = \omega(X_1, \dots, X_p)$  for some  $\omega \in L^2\Lambda^p(\Omega)$  and vector fields  $X_i \in \mathfrak{X}(\Omega)$ , then  $\int_{\Omega} |\omega(\mathbf{X})|^2 dx < \infty$ . Further restricting to a subspace closed under exterior differentiation yields the Sobolev space of differential  $p$ -forms,

$$H\Lambda^p(\Omega) = \{\omega \in L^2\Lambda^p(\Omega) \mid d\omega \in L^2\Lambda^{p+1}(\Omega)\}. \quad (4.8)$$

Finite element approximations of  $H\Lambda^p(\Omega)$  may be characterized by projection maps  $\pi_h$  that ensure the diagram of cochain complexes in Fig. 4.1 commutes—in particular, that  $\pi_h \circ d = d \circ \pi_h$ . Here,  $\Lambda^p(\mathcal{T}_h)$  denotes finite element  $p$ -forms on a triangulation  $\mathcal{T}_h$  of  $\Omega$ , which is defined to have a maximum diameter  $h$  on any given cell. The horizontal arrows form cochain complexes ( $d \circ d = 0$ ), while the vertical projections  $\pi_h$  define isomorphisms of cohomology. Various finite element spaces can be chosen for each  $\Lambda^p(\mathcal{T}_h)$  in the diagram above. However, any such choice must ensure that the sequence of spaces constitutes a cochain complex, and that the finite element problem being studied is solvable and well-posed in those spaces.

A typical choice for  $\Lambda^p(\mathcal{T}_h)$  is given by the space of piecewise polynomial  $p$ -forms of degree  $\leq r$ , denoted  $\mathcal{P}_r\Lambda^p$ . Given a triangular mesh  $\mathcal{T}_h \subset \mathbb{R}^2$ , for example, the space  $\mathcal{P}_1\Lambda^2(T)$  is defined on each triangle  $T \in \mathcal{T}_h$  by the span of 2-forms of the form  $(p_0 + p_1x + p_2y)dx \wedge dy$ .

$$\begin{array}{ccccccc}
0 & \xrightarrow{d} & H\Lambda^0(\Omega) & \xrightarrow{d} & \cdots & \xrightarrow{d} & H\Lambda^n(\Omega) & \xrightarrow{d} & 0 \\
& & \downarrow \pi_h & & & & \downarrow \pi_h & & \\
0 & \xrightarrow{d} & \Lambda^0(\mathcal{T}_h) & \xrightarrow{d} & \cdots & \xrightarrow{d} & \Lambda^n(\mathcal{T}_h) & \xrightarrow{d} & 0
\end{array}$$

Figure 4.1: Given a discretization  $\mathcal{T}_h$  of the smooth manifold  $\Omega$ , each subspace  $H\Lambda^p(\Omega)$  of the continuous cochain complex is projected to a finite element space  $\Lambda^p(\mathcal{T}_h)$ . There are many possible choices, of varying degrees of accuracy, for the spaces of piecewise polynomial finite elements  $\Lambda^p(\mathcal{T}_h)$ . The projections  $\pi_h$  are required to satisfy  $\pi_h \circ d = d \circ \pi_h$ , such that the diagram above is commuting.

Another choice for  $\Lambda^p(\mathcal{T}_h)$  is  $\mathcal{P}_r^- \Lambda^p$ , the ‘trimmed’ piecewise polynomial  $p$ -forms of degree  $\leq r$ . To characterize  $\mathcal{P}_r^- \Lambda^p$ , first denote by  $\mathcal{H}_r \Lambda^p \subset \mathcal{P}_r \Lambda^p$  the homogeneous piecewise polynomial  $p$ -forms of degree *exactly*  $r$ . (For the example  $\mathcal{T}_h \subset \mathbb{R}^2$ ,  $\mathcal{H}_1 \Lambda^2(T)$  is spanned by 2-forms of the form  $(h_1 x + h_2 y) dx \wedge dy$ .) Then further define the *Koszul operator*  $\kappa : \Lambda^p \rightarrow \Lambda^{p-1}$ , an operator that takes the interior product of a  $p$ -form with a radial vector field. In  $\mathbb{R}^3$ , for example,  $\kappa \omega = X_\kappa \lrcorner \omega$  contracts  $\omega$  with the radial vector field  $X_\kappa = x\partial_x + y\partial_y + z\partial_z$ . In general,  $\kappa$  adds one to the polynomial degree of a form, while reducing by one the degree of the form itself.

With this notation,  $\mathcal{P}_r^- \Lambda^p$  may be defined such that

$$\mathcal{P}_r^- \Lambda^p = \mathcal{P}_{r-1} \Lambda^p \oplus \kappa \mathcal{H}_{r-1} \Lambda^{p+1}. \quad (4.9)$$

(For  $\mathcal{T}_h \subset \mathbb{R}^2$  again,  $\mathcal{P}_1^- \Lambda^2(T)$  is spanned by 2-forms of the form  $p_0 dx \wedge dy$  because  $\Lambda^3(\mathcal{T}_h) = \emptyset$  in two dimensions.) Since  $\mathcal{P}_r \Lambda^p = \mathcal{P}_{r-1} \Lambda^p \oplus \mathcal{H}_r \Lambda^p$ , it follows that  $\mathcal{P}_r^- \Lambda^p$  is intermediate to the spaces of piecewise polynomial  $p$ -forms of increasing degree, i.e.

$$\mathcal{P}_{r-1} \Lambda^p \subset \mathcal{P}_r^- \Lambda^p \subset \mathcal{P}_r \Lambda^p. \quad (4.10)$$

On a simplicial (triangular) complex, the space of  $p$ -forms  $\mathcal{P}_1^- \Lambda^p$ —which constitutes the coarsest subfamily of trimmed piecewise polynomials—exactly coincides with the space of Whitney  $p$ -forms [36]. Whitney forms may be defined on an  $n$ -simplex  $T \subset \mathbb{R}^n$  with vertices labeled  $\mathbf{x}_0, \dots, \mathbf{x}_n$ . To describe an arbitrary face (subsimplex) of  $T$  with  $k \leq n$  vertices, let  $\vec{\Sigma}_{0k}^n$  denote the set of increasing maps  $\sigma : \{0, \dots, k\} \rightarrow \{0, \dots, n\}$ . A map  $\sigma \in \vec{\Sigma}_{0k}^n$  thus specifies  $k + 1$  vertices of  $T$ , which define a  $k$ -subsimplex denoted  $f_\sigma \subset T$ . Further recall the barycentric coordinate functions of  $T$ ,  $\{\lambda_0, \dots, \lambda_n\}$ . Each  $\lambda_i(\mathbf{x})$  is defined as the unique linear function on  $T$  satisfying  $\lambda_i(\mathbf{x}_j) = \delta_{ij} \forall j \in [0, n]$ . Finally, the Whitney  $p$ -form on  $T$  associated to the  $p$ -subsimplex  $f_\sigma \subset T$  is denoted  $\phi_\sigma(\mathbf{x})$  and defined by

$$\phi_\sigma = \sum_{i=0}^p (-1)^i \lambda_{\sigma(i)} \left[ d\lambda_{\sigma(0)} \wedge \cdots \wedge \widehat{d\lambda_{\sigma(i)}} \wedge \cdots \wedge d\lambda_{\sigma(p)} \right], \quad (4.11)$$

where the hat signifies that  $d\lambda_{\sigma(i)}$  is omitted.

Since  $\lambda_i$  is linear and vanishes at all vertices except  $\mathbf{x}_i$ , it can be shown that  $\int_{f_\tau} \phi_\sigma = \pm \delta_{\sigma\tau} / p!$  for any  $\sigma, \tau \in \vec{\Sigma}_{0p}^n$ . Up to a factor, therefore, Whitney  $p$ -forms (such as  $\phi_\sigma$ ) and  $p$ -subsimplices (such as  $f_\tau$ ) are dual to one another via integration. As a consequence of this duality, the projection  $\pi_h : \omega \mapsto \sum a_\sigma \phi_\sigma$  of Fig. 4.1—from  $p$ -forms  $\omega \in H\Lambda^p(\Omega)$  to the space  $\mathcal{P}_1^- \Lambda^p$  spanned by Whitney forms on  $\mathcal{T}_h$ —may be determined simply by ensuring that the integrals of  $\omega$  and its discrete counterpart  $\pi_h(\omega) = \sum a_\sigma \phi_\sigma$  agree on each  $p$ -subsimplex  $f_\sigma \in \mathcal{T}_h$ .

More detailed descriptions of cochain-complex-conforming finite element spaces can be found in Refs. [34, 35, 75, 76]. For now, having reviewed some common finite element spaces, notation can now be set for practical calculations in the finite element setting. Given a space of finite element  $p$ -forms  $\Lambda^p(\mathcal{T}_h)$  on  $\mathcal{T}_h$ , a basis of  $N_p$  finite elements can be fixed for  $\Lambda^p(\mathcal{T}_h)$  and organized into the  $N_p \times 1$  vector  $\mathbf{\Lambda}^p$ . The  $i^{\text{th}}$  entry of  $\mathbf{\Lambda}^p$  is a basis element denoted  $\Lambda_i^p \in \Lambda^p(\mathcal{T}_h)$ , which defines a piecewise

polynomial  $p$ -form on  $\mathcal{T}_h$ . Any  $p$ -form  $\mathbf{S} \in \Lambda^p(\mathcal{T}_h)$  may thus be expanded in the  $\Lambda^p$  basis as

$$\mathbf{S}(\mathbf{x}) = \mathbf{s} \cdot \mathbf{\Lambda}^p(\mathbf{x}) = s_i \Lambda_i^p(\mathbf{x}), \quad (4.12)$$

whose individual components are denoted

$$\mathbf{S}(\mathbf{x})_{\mu_1 \dots \mu_p} = \mathbf{s} \cdot \mathbf{\Lambda}^p(\mathbf{x})_{\mu_1 \dots \mu_p} = s_i \Lambda_i^p(\mathbf{x})_{\mu_1 \dots \mu_p}. \quad (4.13)$$

Here,  $\mathbf{s} \in \mathbb{R}^{N_p}$  and Einstein summation convention is used for the repeated  $i$  index. Greek letters denote coordinate indices. In  $\mathbb{R}^3$ , for example, the  $\mu^{\text{th}}$  component of the 1-form basis element  $\Lambda_i^1(\mathbf{x})$  is denoted  $\Lambda_i^1(\mathbf{x})_\mu$  for  $\mu \in \{1, 2, 3\}$ , such that  $\Lambda_i^1(\mathbf{x}) = \Lambda_i^1(\mathbf{x})_\mu dx^\mu$ .

Exterior calculus may be computed in the  $\Lambda^0, \dots, \Lambda^n$  bases by simple matrix multiplication. On  $\mathbb{R}^3$ , for example, where the exterior derivatives of 0-, 1-, and 2-forms can be implemented via matrices that represent the gradient ( $\mathbb{G}$ ), curl ( $\mathbb{C}$ ), and divergence ( $\mathbb{D}$ ), respectively. In Table 4.1, these matrix operators are defined to act on the coefficients of forms. For example, the gradient of the 0-form  $\mathbf{S} = \mathbf{s} \cdot \mathbf{\Lambda}^0$  is computed to be  $d\mathbf{S} = \mathbb{G}\mathbf{s} \cdot \mathbf{\Lambda}^1$ , where the matrix  $\mathbb{G} \in \mathbb{R}^{N_1 \times N_0}$  is defined such that  $d\mathbf{\Lambda}^0 = \mathbb{G}^T \mathbf{\Lambda}^1$ . This definition gives the desired result since

$$d\mathbf{S} = \mathbf{s} \cdot d\mathbf{\Lambda}^0 = \mathbf{s} \cdot \mathbb{G}^T \mathbf{\Lambda}^1 = \mathbb{G}\mathbf{s} \cdot \mathbf{\Lambda}^1. \quad (4.14)$$

It will also be useful to define the *mass matrix* on  $\mathcal{T}_h$  for each basis  $\Lambda^p$  of finite element  $p$ -forms. Specifically, the mass matrix  $\mathbb{M}_p \in \mathbb{R}^{N_p \times N_p}$  of  $\Lambda^p$  is defined by

$$(\mathbb{M}_p)_{ij} = \int_{|\mathcal{T}_h|} d\mathbf{x} \left( \Lambda_i^p, \Lambda_j^p \right)_p = \int_{|\mathcal{T}_h|} \Lambda_i^p \wedge \star \Lambda_j^p. \quad (4.15)$$

$p$ -Form	Abstract d	Matrix d	Definition	Dimensions
$\mathbf{S} = \mathbf{s} \cdot \Lambda^0$	-	-	-	-
$\mathbf{A} = \mathbf{a} \cdot \Lambda^1$	$\mathbf{A} = d\mathbf{S}$	$\mathbf{a} = \mathbb{G}\mathbf{s}$	$\mathbb{G}^T \Lambda^1 = d\Lambda^0$	$\mathbb{G} \in \mathbb{R}^{N_1 \times N_0}$
$\mathbf{B} = \mathbf{b} \cdot \Lambda^2$	$\mathbf{B} = d\mathbf{A}$	$\mathbf{b} = \mathbb{C}\mathbf{a}$	$\mathbb{C}^T \Lambda^2 = d\Lambda^1$	$\mathbb{C} \in \mathbb{R}^{N_2 \times N_1}$
$\mathbf{C} = \mathbf{c} \cdot \Lambda^3$	$\mathbf{C} = d\mathbf{B}$	$\mathbf{c} = \mathbb{D}\mathbf{b}$	$\mathbb{D}^T \Lambda^3 = d\Lambda^2$	$\mathbb{D} \in \mathbb{R}^{N_3 \times N_2}$

Table 4.1: The finite element matrix implementation of d on  $\mathbb{R}^3$ . The property  $d \circ d = 0$  implies that  $\mathbb{C}\mathbb{G} = 0$  and  $\mathbb{D}\mathbb{C} = 0$ .

Here,  $|\mathcal{T}_h|$  denotes the convex hull of  $\mathcal{T}_h$ , and  $(\cdot, \cdot)_p$  denotes the inner product on  $p$ -forms induced by the metric  $g_{\mu\nu}$ , namely

$$\begin{aligned}
(\alpha, \beta)_p &= \frac{1}{p!} \alpha_{\mu_1 \dots \mu_p} \beta^{\mu_1 \dots \mu_p} \\
&= \frac{1}{p!} \alpha_{\mu_1 \dots \mu_p} \beta_{\nu_1 \dots \nu_p} g^{\mu_1 \nu_1} \dots g^{\mu_p \nu_p}.
\end{aligned} \tag{4.16}$$

On  $\mathbb{R}^3$ , for example, Eq. (4.16) defines  $(\alpha, \beta)_p$  for  $p = 1, 2$  simply as the standard inner product  $\alpha \cdot \beta$ . After all, 1- and 2-forms each have three independent components on  $\mathbb{R}^3$  and  $g_{\mu\nu} = \delta_{\mu\nu}$ . Note that  $(\alpha, \beta)_p$  is symmetric, such that  $\mathbb{M}_p^T = \mathbb{M}_p$ . The Hodge star operator  $\star$  is defined by Eq. (4.15), such that  $\alpha \wedge \star\beta = (\alpha, \beta)_p d\mathbf{x}$  for arbitrary  $p$ -forms  $\alpha$  and  $\beta$ , where  $d\mathbf{x}$  denotes the unique volume form that evaluates to unity on positively oriented vectors that are orthonormal with respect to  $g_{\mu\nu}$ . The mass matrix will evidently appear wherever metric information is incorporated via the Hodge star.

### 4.3 Symplectic algorithms

In Section 3.1.1, a symplectic map of the symplectic manifold  $(M, \Omega)$  was introduced as any diffeomorphism  $\phi : M \rightarrow M$  that preserved its symplectic form  $\Omega$ , such that  $\phi^*\Omega = \Omega$ . A *symplectic algorithm* can be understood as the evolution of a symplectic manifold (with finitely many degrees of freedom) whose every discrete timestep is defined by a symplectic map.

### 4.3.1 Conditions for symplecticity

Following [1], such algorithms can be examined on the symplectic manifold  $\mathbb{R}^{2n}$  of phase space, coordinatized by  $\mathbf{z} = [\mathbf{q}; \mathbf{p}]$  for  $\mathbf{q}, \mathbf{p} \in \mathbb{R}^n$ . The symplectic 2-form  $\Omega$  in the basis  $(\partial_{\mathbf{q}}, \partial_{\mathbf{p}})$  induced by this coordinatization can be defined by a higher dimensional matrix generalization of Eq. (3.7)

$$\mathbb{J} = \begin{bmatrix} \mathbb{0}_n & \mathbb{1}_n \\ -\mathbb{1}_n & \mathbb{0}_n \end{bmatrix}, \quad (4.17)$$

where  $\mathbb{1}_n$  denotes the  $n \times n$  identity matrix, and  $\mathbb{0}_n$  denotes the corresponding null matrix. Thus,  $\Omega$  can be evaluated by

$$\Omega(X, Y) = X^T \mathbb{J} Y \quad (4.18)$$

$\forall X, Y \in \Gamma(T\mathbb{R}^{2n})$ .

In this notation, a linear map  $A : \mathbb{R}^{2n} \rightarrow \mathbb{R}^{2n}$  is symplectic if

$$A^T \mathbb{J} A = \mathbb{J}, \quad (4.19)$$

since this condition ensures that

$$(A^* \Omega)(X, Y) = \Omega(A_* X, A_* Y) = \Omega(AX, AY) = X^T A^T \mathbb{J} AY = X^T \mathbb{J} Y = \Omega(X, Y). \quad (4.20)$$

(This calculation uses the fact that  $A_* X = AX$  for a linear map  $A$ .) For a nonlinear differential mapping  $A : \mathbb{R}^{2n} \rightarrow \mathbb{R}^{2n}$  such that  $A : \mathbf{z}_0 \mapsto \mathbf{z}$ , a generalization of the

symplecticity condition of Eq. (4.19) is possible, namely

$$\left(\frac{\partial \mathbf{z}}{\partial \mathbf{z}_0}\right)^T \mathbb{J} \left(\frac{\partial \mathbf{z}}{\partial \mathbf{z}_0}\right) = \mathbb{J}, \quad (4.21)$$

where  $\frac{\partial \mathbf{z}}{\partial \mathbf{z}_0}$  denotes the Jacobian of  $A$ . This follows from the same calculation as Eq. (4.20) after simply substituting  $A_*X = \left(\frac{\partial \mathbf{z}}{\partial \mathbf{z}_0}\right)X$ —as derived in Eq. (2.37).

Note that, by Darboux’s theorem, a symplectic form  $\Omega$  can always be made to locally take the form of  $\mathbb{J}$ , so the above results can be generalized. Lastly, from Eqs. (4.19) and (4.21), it immediately follows that the composition of two symplectic maps is also symplectic.

### 4.3.2 Volume preservation

One immediate consequence of such an algorithm is its preservation of volume in phase space. For example, in two dimensions ( $n = 1$ ), the area of a parallelogram formed by the vectors  $v$  and  $w$  is given by the cross product,  $|v \times w|$ . It is readily seen that in two dimensions the matrix  $\mathbb{J}$  also computes this cross product:  $|v \times w| = |v^T \mathbb{J} w|$ . Under evolution by a symplectic map  $A$  as in Eq. (4.20), therefore, this area is invariant. Similarly, in  $2n$  dimensions, areas in each of the  $n$  planes coordinatized by  $(q_i, p_i)$  are preserved by  $A$ . In fact, due to the distributivity of the pullback over wedge products—as noted in Eq. (2.56)—the total phase space volume  $2n$ -form, defined by

$$\Omega^n = \Omega \wedge \cdots \wedge \Omega \quad (4.22)$$

is preserved by  $A$ . Similarly, arbitrary  $k$ -fold wedge products— $\{\Omega, \Omega \wedge \Omega, \cdots\}$ —are invariant under  $A$ , giving rise to the preservation in symplectic algorithms of all

*Poincaré invariants* [77], which include integrals of the form

$$\left\{ \int \int \sum_i dq_i dp_i \ , \ \int \int \int \int \sum_{i \neq j} dq_i dp_i dq_j dp_j \ , \ \dots \right\} \quad (4.23)$$

over any appropriate even-dimensional surface.

### 4.3.3 Examples of symplectic algorithms

The condition of Eq. (4.21) affords a means to rapidly test the symplecticity of various algorithms, as will now be demonstrated.

#### Symplectic Euler

A simple example of a symplectic algorithm is the symplectic Euler algorithm, which modifies the standard Euler method for the ODE  $\dot{y} = f(y)$ , namely  $y_{n+1} = y_n + hf(y_n)$  with stepsize  $h$ . For any Hamiltonian  $H(q, p)$  on  $\mathbb{R}^2$  phase space, the time advance of the symplectic Euler method is given by [1]:

$$\begin{aligned} p_{n+1} &= p_n - hH_{,q}(q_n, p_{n+1}) \\ q_{n+1} &= q_n + hH_{,p}(q_n, p_{n+1}) \end{aligned} \quad (4.24)$$

where  $H_{,q}$  and  $H_{,p}$  denote partial derivatives of  $H(q, p)$ , and where the subscript  $n \in \mathbb{Z}$  denotes timesteps separated by time interval  $h$ . The symplectic Euler method is generally *implicit*, since the right hand sides of Eq. (4.24) depend upon the variables being solved for on the left. It should be noted, however, that this dependence drops out for separable Hamiltonians of the form  $H(q, p) = V(q) + K(p)$ , for which the method is *explicit*.

To see that Eq. (4.24) defines a symplectic algorithm, note that its Jacobian

$\partial(q_{n+1}, p_{n+1})/\partial(q_n, p_n)$  follows from differentiating Eq. (4.24) to find

$$\begin{bmatrix} 1 & -hH_{,pp} \\ 0 & 1 + hH_{,qp} \end{bmatrix} \begin{bmatrix} \frac{\partial q_{n+1}}{\partial q_n} & \frac{\partial q_{n+1}}{\partial p_n} \\ \frac{\partial p_{n+1}}{\partial q_n} & \frac{\partial p_{n+1}}{\partial p_n} \end{bmatrix} = \begin{bmatrix} 1 + hH_{,pq} & 0 \\ -hH_{,qq} & 1 \end{bmatrix}. \quad (4.25)$$

Here, partial derivatives ( $H_{,qq}, H_{,qp}, H_{,pp}$ ) are taken with respect to  $q_n$  and  $p_{n+1}$ . Solving for the Jacobian, it is readily confirmed to satisfy the symplecticity condition of Eq. (4.21). Symplectic Euler is a first order method, with error scaling as  $\mathcal{O}(h)$ .

## Leapfrog

Another classic example of a symplectic algorithm is the leapfrog algorithm (or Störmer-Verlet scheme [78]). Its first appearance, in fact, dates back to Newton's proof of Kepler's Second Law in the *Principia Mathematica* [79]. For any Hamiltonian  $H(q, p)$  on  $\mathbb{R}^2$  phase space, the time advance of the leapfrog method is given by:

$$\begin{aligned} p_{n+\frac{1}{2}} &= p_n - \frac{h}{2} H_{,q} \left( q_n, p_{n+\frac{1}{2}} \right) \\ q_{n+1} &= q_n + \frac{h}{2} \left[ H_{,p} \left( q_n, p_{n+\frac{1}{2}} \right) + H_{,p} \left( q_{n+1}, p_{n+\frac{1}{2}} \right) \right] \\ p_{n+1} &= p_{n+\frac{1}{2}} - \frac{h}{2} H_{,q} \left( q_{n+1}, p_{n+\frac{1}{2}} \right). \end{aligned} \quad (4.26)$$

For separable Hamiltonians, like symplectic Euler, leapfrog is an explicit algorithm. It is also a second order method, with error scaling as  $\mathcal{O}(h^2)$ .

## Splitting Methods

Another class of symplectic algorithms, which is crucial to the work in the ensuing Section 4.4, is the splitting method. Due to their ease of computation, splitting methods offer an appealing algorithmic implementation of many Hamiltonian systems [for example, see 12]. In effect, a splitting method splits a system's Hamiltonian  $H$

into some finite number  $n_H$  of ‘sub-Hamiltonians’  $\{H_i\}$  such that

$$H = \sum_{i=1}^{n_H} H_i. \quad (4.27)$$

The system’s dynamical variables  $\mathbf{u}$  are then evolved by each subsystem individually, arranged in a sequence chosen to minimize discretization error, e.g.

$$\begin{aligned} \mathbf{u}(t + \Delta t) &= \exp(\Delta t H) \mathbf{u}(t) \\ &\approx \exp\left(\frac{\Delta t}{2} H_1\right) \exp(\Delta t H_2) \exp\left(\frac{\Delta t}{2} H_1\right) \mathbf{u}(t), \end{aligned} \quad (4.28)$$

where  $n_H = 2$  subsystems are schematically represented,  $H = H_1 + H_2$ , arranged in a second-order Strang splitting [80].

The advantage afforded by this subdivision of the Hamiltonian is that its subsystems  $\{H_i\}$  are often more easily integrated individually than the full system  $H$ . Each subsystem can be integrated by a symplectic method, so that the full splitting method is symplectic. In fact, each sub-Hamiltonian  $H_i$  can at times be made sufficiently simple to allow its *exact* integration, without any discrete approximation. Explicit examples of this exact evolution will be seen in the Vlasov-Maxwell splitting methods detailed in Chapter 5.

Splitting methods can be constructed to arbitrarily high order. The simplest, first-order method is known as a Lie-Trotter splitting. Following the notation of [1] and denoting the map of a given sub-Hamiltonian by  $\varphi_h^{[i]} = \exp(hH_i) \forall i \in [1, n_H]$ , the Lie-Trotter splitting [81] is defined by

$$\Phi_h^{[L]} = \varphi_h^{[1]} \circ \dots \circ \varphi_h^{[n_H]}. \quad (4.29)$$

Further defining the *adjoint* of a method

$$\Phi_h^* = \Phi_{-h}^{-1}, \quad (4.30)$$

which has the effect of reversing its sequence of mappings, the second order Strang splitting [80] in Eq. (4.28) above can be rewritten

$$\Phi_h^{[S]} = \Phi_{h/2}^{[L]} \circ \Phi_{h/2}^{[L]*} = \varphi_{h/2}^{[1]} \circ \varphi_h^{[2]} \circ \varphi_{h/2}^{[1]}. \quad (4.31)$$

In greater generality, given an  $\mathcal{O}(h)$  method  $\Phi_h$  (such as  $\Phi_h^{[L]}$  above), a splitting method  $\hat{\Phi}_h$  of order  $p + 1$  can be defined by [1]

$$\begin{aligned} \hat{\Phi}_h &= \Phi_{\alpha_s h} \circ \Phi_{\beta_s h}^* \circ \cdots \circ \Phi_{\beta_2 h}^* \circ \Phi_{\alpha_1 h} \circ \Phi_{\beta_1 h}^* \\ 1 &= \sum_{i=1}^s (\alpha_i + \beta_i) \\ 0 &= \sum_{i=1}^s \left[ (-1)^p \beta_i^{p+1} + \alpha_i^{p+1} \right]. \end{aligned} \quad (4.32)$$

The coefficients  $\alpha_i, \beta_i$  may also be further optimized to reduce error.

## 4.4 Gauge-compatible splitting methods

A splitting method's exact integration for sufficiently simplified subsystems offers a considerable opportunity for the construction of structure-preserving symplectic algorithms. In particular, the momentum map will now be reconsidered—along with its associated conservation laws—in the context of such methods.

What is the status of the momentum map  $\mu$  in splitting algorithms? A sufficient condition for the exact preservation of  $\mu$  is straightforward to state. In particular, suppose that each sub-Hamiltonian of a splitting method is gauge invariant—that is,

invariant under the group action of some group  $G$ —

$$\Phi_g^* H_i = H_i \quad \forall i \text{ and } g \in G. \quad (4.33)$$

Then, ‘differentiating with respect to  $g$ ’—that is, setting  $g = \exp(sA)$  and taking  $\left. \frac{d}{ds} \right|_{s=0}$ —it follows by the same argument of Eq. (3.29) that  $\dot{\mu} = 0$  in each Hamiltonian subsystem, where  $\mu$  is the total system’s momentum map associated with the group action  $\Phi_g$ .

As previously noted, this claim follows simply from the observation that  $\mu$  is an object defined by its Poisson manifold  $(M, \{\cdot, \cdot\})$ , separate and apart from the Hamiltonian defined on that manifold.  $\mu$  is therefore preserved along the flow generated by *any* gauge-invariant function. Consequently, if each sub-Hamiltonian is gauge invariant and its flow is exactly integrated, then the momentum map is exactly preserved by its evolution during each discrete time step. This result is now summarized as a theorem.

**Theorem.** Let  $\Phi$  be a canonical group action of a Lie group  $G$  on Poisson manifold  $M$  with momentum map  $\mu$ , and let  $H : M \rightarrow \mathbb{R}$  satisfy  $\Phi_g^* H = H$ ,  $\forall g \in G$ . Suppose a splitting method  $H = \sum_{i=1}^N H_i$  satisfies:

- (1)  $\Phi_g^* H_i = H_i, \forall i \text{ and } g \in G;$
- (2) subsystem  $H_i$  is solved exactly  $\forall i$ .

Then  $\mu$  is exactly preserved by the splitting method—that is,  $\dot{\mu} = 0$ .

Such algorithms are hereafter referred to as *gauge-compatible splitting methods*, or GCSMs. Gauge-compatible splitting methods enjoy a significant advantage over alternative Hamiltonian integrators, in that they exactly preserve the gauge structure of the systems they simulate via the momentum map. As such, they preserve exact

conservation laws, even in discrete time.

## 4.5 Variational algorithms

Another important class of structure-preserving algorithms are *variational algorithms*—those derived by applying a variational principle to a discretized action in the Lagrangian formalism. Closely following [40, 45, 82], some important properties of variational systems and their algorithms are now considered.

### 4.5.1 Noether’s theorems in a finite difference formalism

It will first be demonstrated that the derivation of Noether’s theorems, included in Section 3.2.5 for continuous spacetime variational systems, has a remarkably parallel counterpart in finite difference variational systems. Aside from replacing the infinitesimal calculus that is used to characterize an action (via integration) or a divergence (via differentiation), for example, little else in the derivation need be modified.

More specifically, rather than constructing operators out of derivatives in terms of independent coordinate variables, finite difference Lagrangians depend on shift operators [40],

$$S_i : n^j \mapsto n^j + \delta_i^j. \tag{4.34}$$

Here,  $\mathbf{n} = (n^1, \dots, n^r) \in \mathbb{Z}^r$  denotes an integer-labeled vertex of an  $r$ -dimensional cubic lattice. A forward difference can then be simply constructed by

$$D_i = S_i - \mathbb{1}, \tag{4.35}$$

where  $\mathbb{1}$  denotes the identity map.

An action in this formalism is defined by a sum over vertices, that is,

$$\mathcal{S}[u] = \sum_{\mathbf{n}} L(\mathbf{n}, [u]) \quad (4.36)$$

where  $[u] = \{u^\ell(\mathbf{n})\}$  now denotes the set of dependent variables at  $\mathbf{n}$  and finitely many of their shifts. Equations of motion for such a Lagrangian are then simply given by

$$\mathbf{E}_\ell(L) = \mathbf{S}_{-J} \left[ \frac{\partial L}{\partial(\mathbf{S}_J u^\ell)} \right] = 0 \quad (4.37)$$

where  $J$  denotes an arbitrary shift multi-index whose repetition in the above expression indicates that it is summed over.

Note that the discrete Euler operator, which operates on the Lagrangian, is equivalent to taking a partial derivative of the action  $\mathcal{S}[u]$  with respect to  $u^\ell(\mathbf{n})$  at a fixed vertex on the lattice. That is  $\mathbf{E}_\ell(L) = \partial\mathcal{S}[u]/\partial u^\ell(\mathbf{n})$ —a fact that shall be put to use in the exploration of Noether’s second theorem in a discrete exterior calculus formalism in Section 5.4. Moreover, it can be readily shown [39] that, in analogy with its continuous counterpart,  $\mathbf{E}_\ell \circ \text{Div} = 0$  for the discrete divergence operator  $\text{Div}A = \mathbf{D}_i A^i$ .

Symmetries of these discrete equations of motion have a form very much like the (prolonged) symmetry vector defined in Eq. (3.76). In particular, the prolongation of a symmetry of a finite difference Lagrangian can be defined by

$$Y = \mathbf{S}_J Q^\ell(\mathbf{n}, [\mathbf{u}]) \frac{\partial}{\partial \mathbf{S}_J u^\ell} \quad (4.38)$$

where  $Q^\ell$  denote, as before, the characteristics of  $Y$ .

As in Eq. (3.85) for the continuous case, Eq. (4.38) is said to define a *variational symmetry* if

$$Y(L) = \mathbf{D}_i A^i(\mathbf{n}, [u]) = \text{Div}A \quad (4.39)$$

for some  $r$ -tuple  $A[u] = (A^1[u], \dots, A^r[u])$ .

Finally, summing Eq. (4.39) by parts [40] reveals the discrete counterpart to the symmetry criterion of Eq. (3.87), namely:

$$Q^\ell E_\ell(L) = D_i B^i(\mathbf{n}, [\mathbf{u}]) \quad (4.40)$$

with all operators understood to be discrete.

As in the continuous case, this expression of the symmetry condition immediately leads to Noether's first and second theorems. After all, the left hand side vanishes on shell, so that the right hand side constitutes a discrete local conservation law. Moreover, if the characteristics of  $Y$  are dependent on a function with arbitrary dependence on the lattice—e.g.,  $Q^\ell[u; \boldsymbol{\lambda}(\mathbf{n})]$ —then the discrete Euler operator associated to  $\boldsymbol{\lambda}$  can be applied to Eq. (4.40) to derive an off-shell discrete differential identity satisfied by the equations of motion.

## 4.5.2 Lagrangian systems' symplectic structure

Having described some of the properties of symplectic dynamical systems in the previous sections, it is all the more impactful to note that Lagrangian systems preserve a symplectic structure as well.

Hamilton's principle, as seen in Section 3.2.4, holds that the trajectory of a variational system between two fixed points lies along an extremal of its action. Equations of motion in that section were therefore derived by considering variations of the system that were independent of the boundary. To understand the properties of variational algorithms, however, it will be critical to revisit variations that include the boundaries of the trajectory.

Following [45, 82], consider the typical setting of Lagrangian mechanics with configuration space  $Q$  and a first-order Lagrangian  $L = L(q, \dot{q})$  that constitutes a

map  $L : TQ \rightarrow \mathbb{R}$ . Here it will be convenient to define the action  $\mathcal{S}(q) : \mathcal{C}(q) \rightarrow \mathbb{R}$  as a map on *path space*  $\mathcal{C}(q)$ , a smooth manifold defined by the set of paths  $\mathcal{C}(q) = \{q : [0, T] \rightarrow Q \mid q \text{ is a } C^2 \text{ curve}\}$  such that

$$\mathcal{S}(q) = \int_0^T L(q(t), \dot{q}(t)) dt. \quad (4.41)$$

If the variation of  $\mathcal{S}(q)$ —derived analogously to Eq. (3.80)—is now computed  $\forall \delta q \in T_q \mathcal{C}(Q)$  (*including* boundary variations), the resulting variation is given by

$$d\mathcal{S}(q) \cdot \delta q = \int_0^T \mathbf{E}_{q^i}(L[q(t)]) \cdot \delta q^i(t) dt + \left[ \frac{\partial L}{\partial \dot{q}^i} \delta q^i \right]_0^T. \quad (4.42)$$

The new boundary term arises from the integration by parts of the variation. It can be regarded as a 1-form—the so called *Lagrangian 1-form*  $\Theta_L \in T^*(TQ)$  defined by

$$\Theta_L = \frac{\partial L}{\partial \dot{q}^i} dq^i \quad (4.43)$$

—evaluated on  $(\delta q, \delta \dot{q}) \in T_{(q, \dot{q})}(TQ)$ .

Now consider a restriction of the path space  $\mathcal{C}(Q)$  to its *solution space*  $\mathcal{C}_L(Q) \subset \mathcal{C}(Q)$  comprised of solutions to the Euler-Lagrange equations, that is  $\mathcal{C}_L(Q) = \{q \mid \mathbf{E}_{q^i}(L[q(t)]) = 0 \ \forall i\}$ . Since a solution is uniquely determined by its initial conditions  $(q_0, \dot{q}_0)$ , one can formally identify  $\mathcal{C}_L(Q)$  with  $TQ$ .

One may thus define  $v_0 = (q_0, \dot{q}_0) \in T_{q_0}Q$  and denote the restricted action  $\hat{\mathcal{S}}(v_0) = \mathcal{S}(q)$ . Furthermore, one may denote the evolution of the system from its state at  $t = 0$  to its state at  $t = T$  according to the Lagrangian dynamics by the map  $F_L : TQ \rightarrow TQ$ . Then, on the restricted domain of  $\mathcal{C}_L(Q)$ , the first term of Eq. (4.42)

vanishes and leaves

$$\begin{aligned} d\hat{\mathcal{S}}(v_0) \cdot w &= \Theta_L \Big|_{\dot{q}(T)} (F_{L*} w) - \Theta_L \Big|_{v_0} (w) \\ &= (F_L^* \Theta_L - \Theta_L) \Big|_{v_0} (w) \end{aligned} \tag{4.44}$$

$\forall w \in T_{v_0}(TQ)$ . Taking another exterior derivative and recalling that it naturally commutes with pullbacks, Eq. (4.44) implies

$$0 = d^2 \hat{\mathcal{S}} = F_L^* \Omega_L - \Omega_L \tag{4.45}$$

where  $\Omega_L = d\Theta_L$ . This is a statement of the exact preservation of the so-called *Lagrangian symplectic form*, which, for a Lagrangian system constructed from the configuration space  $Q$ , is given by

$$\Omega_L(q, \dot{q}) = \frac{\partial^2 L}{\partial q^i \partial \dot{q}^j} dq^i \wedge d\dot{q}^j + \frac{\partial^2 L}{\partial \dot{q}^i \partial \dot{q}^j} d\dot{q}^i \wedge d\dot{q}^j. \tag{4.46}$$

# 5

## Applications to Vlasov-Maxwell Particle-in-Cell Algorithms

This chapter marks a culmination of those preceding it, in that it synthesizes the formalism developed in Chapter 3 to explore the gauge structure of dynamical systems, with the elements developed in Chapter 4 that preserve gauge structure in discrete algorithms, to study and construct gauge-structure-preserving particle-in-cell algorithms. This chapter is comprised of original contributions.

### 5.1 Overview

Particle-in-cell (PIC) methods have long been an indispensable tool in studies of plasma physics [29–31, 83–102]. Even before structure-preserving algorithms began to be more widely explored, the literature counted several examples of PIC methods that had been engineered to exactly conserve charge by the use of various sophisticated numerical techniques [103–106].

In recent years, however, elegant PIC methods have been developed that preserve the gauge symmetry of the plasmas they simulate, not as the result of bespoke numerical methods, but as a natural consequence of preserving their systems’ geometric

structure. It was Squire *et al.* [3] that first derived an exactly charge-conserving variational PIC scheme by imposing gauge symmetry on a discrete action. Several gauge-symmetric algorithms have since followed [4–28], especially in the form of Hamiltonian PIC schemes. Many of these references note that the gauge symmetry of their algorithms guarantees exact charge conservation, but this fact is often unproven; the associated conservation laws are not always stated, let alone systematically derived. The absence of such derivations motivates a rigorous study of algorithmic conservation laws in PIC methods.

Indeed, most of the literature’s recent structure-preserving Hamiltonian PIC methods employ a non-canonical Poisson structure to describe particle degrees of freedom  $(\mathbf{X}, \mathbf{V})$  and discrete electromagnetic fields  $(\mathbf{E}, \mathbf{B})$  [7–10, 12–18, 22–24, 26, 27]. This approach hides from view the gauge symmetry of the Vlasov-Maxwell system and the simplicity of its canonical Poisson structure, which is characterized by the electromagnetic potential  $\mathbf{A}$  and its conjugate momentum  $\mathbf{Y} \sim d\mathbf{A}/dt$ . The process of ‘hiding’ this gauge symmetry may be formally regarded as the Poisson reduction of the Vlasov-Maxwell system [19, 57–59], which strips out gauge symmetry to reduce canonical coordinates  $(\mathbf{A}, \mathbf{Y}, \mathbf{X}, \mathbf{P})$  to their non-canonical counterparts  $(\mathbf{E}, \mathbf{B}, \mathbf{X}, \mathbf{V})$ .

In this chapter, the methods developed in this thesis are applied to the study and construction of PIC algorithms that preserve gauge structure. Charge conservation laws are derived in Hamiltonian splitting and variational algorithms from first principles. In so doing, the requirements for gauge-symmetric codes to be charge conserving are elucidated, and a general template for the derivation of conservation laws from the gauge symmetry of Hamiltonian and Lagrangian algorithms is found.

The effectiveness of gauge-compatible splitting methods (GCSMs) is demonstrated in practice by the construction of two new GCSMs, and numerical results are presented. These effort highlights the practical usefulness of solving for the momentum map in Hamiltonian algorithms, for example, in determining the correct specification

of their initial conditions.

This chapter appears in three sections, which may be read independently:

- Section 5.2, following Glasser and Qin [19], constructs a GCSM for the canonical Vlasov-Maxwell system on a cubic mesh, and studies its symplectic reduction. Rather than imposing an interpolation scheme a priori, this section aims to preserve gauge structure and discovers the prerequisites necessary to achieve it. (The required properties (re-)discovered are essentially those of the Whitney forms [36] and their generalizations.)
- Section 5.3, following Glasser and Qin [28], constructs another GCSM using finite element exterior calculus, suitable for simulation on an unstructured mesh, and presents results from its numerical implementation in simulations of Landau damping and the Weibel instability.
- Section 5.4, following Glasser and Qin [19], demonstrates the systematic derivation of an exact charge conservation law for the Lagrangian variational PIC method of [3]. This conservation law is discovered from the system's local gauge symmetry using Noether's second theorem (N2T) in the setting of discrete exterior calculus (DEC) [32, 33], leveraging the formalism of Hydon and Mansfield [40]. This effort demonstrates the usefulness of discovering off-shell differential identities in discrete, degenerate Lagrangian systems, whose continuity equations and conservation laws may not be known a priori.

## 5.2 A GCSM for PIC simulations on a cubic mesh and its symplectic reduction

### 5.2.1 A discrete canonical Poisson structure for the Vlasov-Maxwell system

In this section, a GCSM PIC method is constructed from the canonical Poisson structure of the Vlasov-Maxwell system. The resulting algorithm can be viewed as synthesis of Xiao *et al.* [8] and Qin *et al.* [11]. The latter of these references implements a symplectic-Euler integrator for the ‘unreduced,’ canonical Poisson bracket of Eq. (3.39), while the former implements a splitting method for the ‘reduced’ bracket of Eq. (3.62). Adapting elements from each, a gauge-compatible splitting method is discovered for the unreduced bracket of Eq. (3.39) and, in so doing, demonstrates the merit of this new class of splitting methods. The result is an explicit-time-advance, canonical, locally charge-conserving PIC method, whose momentum map and conservation law shall be systematically derived.

In Qin *et al.* [11], a Klimontovich-Maxwell PIC method is derived from the unreduced bracket of Eq. (3.39) by specifying the following form for the distribution function  $f(\mathbf{x}, \mathbf{p})$  of  $L$  particles in phase space, as in Eq. (3.96):

$$f(\mathbf{x}, \mathbf{p}) = \sum_{i=1}^L \delta^{(3)}(\mathbf{x} - \mathbf{X}_i) \delta^{(3)}(\mathbf{p} - \mathbf{P}_i). \quad (5.1)$$

Here,  $(\mathbf{X}_i, \mathbf{P}_i)$  denotes the dynamical coordinates of particle  $i$  in phase space. The fields  $\mathbf{A}$  and  $\mathbf{Y}$  introduced in the Poisson bracket of Marsden and Weinstein [59] (see Eq. (3.39)) are also discretized on a (three-dimensional) spatial lattice and denoted

$(\mathbf{A}_n, \mathbf{Y}_n)$  at lattice site  $n$ . The interpolation of  $\mathbf{A}$  will also be required,

$$\mathbf{A}(\mathbf{x}) = \sum_{n=1}^N \mathbf{A}_n W_{\sigma_1}(\mathbf{x} - \mathbf{x}_n) \quad (5.2)$$

where  $n$  is an index over all  $N$  lattice sites and  $W_{\sigma_1}$  is an (as yet unspecified) interpolation function for  $\mathbf{A}$ .

A Poisson bracket for this discrete system simply follows from the canonical symplectic structure of its variables. In particular, the symplectic manifold

$$M_d = T^*X \times T^*Q, \quad (5.3)$$

is defined, where  $X = \mathbb{R}^{3L}$  is the space of particle position coordinates and  $Q = \mathbb{R}^{3N}$  is the space of vector potentials on the lattice, such that  $T^*X = \{(\mathbf{X}_i, \mathbf{P}_i)\}$  and  $T^*Q = \{(\mathbf{A}_n, \mathbf{Y}_n)\}$ . A point  $m \in M_d$  correspondingly specifies  $(\mathbf{X}_i, \mathbf{P}_i, \mathbf{A}_n, \mathbf{Y}_n) \forall i, n$  (where the subscript  $d$  denotes discretization).

The Poisson bracket for this symplectic manifold therefore takes its usual Darboux-coordinate form

$$\begin{aligned} \{\{F, G\}\}_d[\mathbf{X}_i, \mathbf{P}_i, \mathbf{A}_n, \mathbf{Y}_n] &= \sum_{i=1}^L \left( \frac{\partial F}{\partial \mathbf{X}_i} \cdot \frac{\partial G}{\partial \mathbf{P}_i} - \frac{\partial G}{\partial \mathbf{X}_i} \cdot \frac{\partial F}{\partial \mathbf{P}_i} \right) \\ &+ \sum_{n=1}^N \left( \frac{\partial F}{\partial \mathbf{A}_n} \cdot \frac{\partial G}{\partial \mathbf{Y}_n} - \frac{\partial G}{\partial \mathbf{A}_n} \cdot \frac{\partial F}{\partial \mathbf{Y}_n} \right). \end{aligned} \quad (5.4)$$

Observe that, unlike its continuous counterpart in Eq. (3.39), the bracket of Eq. (5.4) is non-degenerate; it defines  $M_d$  not only as a Poisson manifold, but as a symplectic manifold.

The discrete Hamiltonian of Qin *et al.* [11] is derived from Eq. (3.40) by substi-

tuting the Klimontovich distribution of Eq. (5.1), yielding

$$\begin{aligned}
H_d[\mathbf{X}_i, \mathbf{P}_i, \mathbf{A}_n, \mathbf{Y}_n] = & \frac{1}{2} \sum_{i=1}^L \left[ \mathbf{P}_i^2 - 2\mathbf{P}_i \cdot \sum_{n=1}^N \mathbf{A}_n W_{\sigma_1}(\mathbf{X}_i - \mathbf{x}_n) \right. \\
& \left. + \sum_{m,n=1}^N \mathbf{A}_m \cdot \mathbf{A}_n W_{\sigma_1}(\mathbf{X}_i - \mathbf{x}_m) W_{\sigma_1}(\mathbf{X}_i - \mathbf{x}_n) \right] + \frac{1}{2} \sum_{n=1}^N \left[ \mathbf{Y}_n^2 + |\nabla_d^+ \times \mathbf{A}|_n^2 \right],
\end{aligned} \tag{5.5}$$

after explicitly expanding terms of the form  $|\mathbf{P}_i - \mathbf{A}(\mathbf{X}_i)|^2$  using Eq. (5.2). Here, the operator  $(\nabla_d^\pm \times)_n$  represents a discrete curl, defined by

$$(\nabla_d^\pm \times \mathbf{A})_n := \pm \begin{pmatrix} \frac{A_{i,j\pm 1,k}^3 - A_{i,j,k}^3}{\Delta y} - \frac{A_{i,j,k\pm 1}^2 - A_{i,j,k}^2}{\Delta z} \\ \frac{A_{i,j,k\pm 1}^1 - A_{i,j,k}^1}{\Delta z} - \frac{A_{i\pm 1,j,k}^3 - A_{i,j,k}^3}{\Delta x} \\ \frac{A_{i\pm 1,j,k}^2 - A_{i,j,k}^2}{\Delta x} - \frac{A_{i,j\pm 1,k}^1 - A_{i,j,k}^1}{\Delta y} \end{pmatrix} \tag{5.6}$$

for  $n = (i, j, k)$ .

## 5.2.2 Examining its gauge symmetry and momentum map

The gauge symmetry of this discrete Hamiltonian system can now be described. The group action  $\Phi_f$  on  $M_d$  is defined by analogy with Eq. (3.49)

$$\Phi_f(\mathbf{X}_i, \mathbf{P}_i, \mathbf{A}_n, \mathbf{Y}_n) = \left( \mathbf{X}_i, \left[ \mathbf{P}_i - \nabla_d^+ f(\mathbf{X}_i) \right], \left[ \mathbf{A}_n - (\nabla_d^+ f)_n \right], \mathbf{Y}_n \right), \tag{5.7}$$

where

$$\nabla_d^+ f(\mathbf{x}) = \sum_{n=1}^N (\nabla_d^+ f)_n W_{\sigma_1}(\mathbf{x} - \mathbf{x}_n) \tag{5.8}$$

and where  $(\nabla_d^\pm)_n$  is a discrete gradient defined by

$$(\nabla_d^\pm f)_n := \pm \begin{pmatrix} \frac{f_{i\pm 1,j,k} - f_{i,j,k}}{\Delta x} \\ \frac{f_{i,j\pm 1,k} - f_{i,j,k}}{\Delta y} \\ \frac{f_{i,j,k\pm 1} - f_{i,j,k}}{\Delta z} \end{pmatrix}. \quad (5.9)$$

Note that  $\nabla_d^\pm \times \nabla_d^\pm = 0$  as an operator. (If the  $\pm$  signs agree, this relation holds identically; if they disagree, it holds only after a summation over lattice points,  $\sum_n$ .) Furthermore—in contrast with Eqs. (3.49)–(3.50)— $\mathbf{P}_i$  and  $\mathbf{A}_n$  are shifted in the same direction in Eq. (5.7), reflecting the fact that  $\mathbf{p}$  and  $\mathbf{P}_i$  have opposite signs in Eq. (5.1) when the transformation of Eq. (3.50) is reinterpreted as a transformation of  $\mathbf{P}_i$ .

The function  $f$  appearing in the group action of Eq. (5.7) is to be understood as a scalar function defined only at lattice points. In particular,  $f \in \mathcal{F}_d$  is a group element of the set  $\mathcal{F}_d$  of discrete scalar functions with an abelian composition law of addition. Its Lie algebra  $\mathfrak{f}_d$  is also the set of discrete scalar functions on the lattice, while its dual  $\mathfrak{f}_d^*$  is the set of densities, which pair to elements of  $\mathfrak{f}_d$  by summing over pointwise products

$$\langle \alpha, \phi \rangle := \sum_{n=1}^N \alpha_n \phi_n \quad \forall \alpha \in \mathfrak{f}_d^*, \phi \in \mathfrak{f}_d. \quad (5.10)$$

It must be verified that the group action is canonical, a task best approached infinitesimally (as described in Eq. (3.10)). In particular, it can be checked that the following infinitesimal form of  $\{\{\Phi_f^* F, \Phi_f^* G\}\}_d = \Phi_f^* \{\{F, G\}\}_d$  holds:

$$\begin{aligned} & \left\{ \left\{ -\nabla_d^+ \phi(\mathbf{X}_i) \cdot \frac{\partial F}{\partial \mathbf{P}_i} - \nabla_d^+ \phi_n \cdot \frac{\partial F}{\partial \mathbf{A}_n}, G \right\} \right\}_d - (F \leftrightarrow G) \\ & = -\nabla_d^+ \phi(\mathbf{X}_i) \cdot \frac{\partial \{\{F, G\}\}_d}{\partial \mathbf{P}_i} - \nabla_d^+ \phi_n \cdot \frac{\partial \{\{F, G\}\}_d}{\partial \mathbf{A}_n}, \end{aligned} \quad (5.11)$$

where summation over repeated indices is implicit. After applying Eq. (5.4) to eval-

uate each bracket, Eq. (5.11) is seen to be true only when  $\nabla \times \nabla_d^+ \phi(\mathbf{X}_i) = 0$ . This requires the operator relation

$$\nabla \times \nabla_d^+ = 0. \quad (5.12)$$

Here,  $\nabla \equiv \partial_{\mathbf{x}_i}$  is a continuous spatial gradient.

Eq. (5.12) therefore necessitates the following condition on the interpolation function  $W_{\sigma_1}$ :

$$\sum_{n=1}^N (\nabla_d^+ \phi)_n W_{\sigma_1}(\mathbf{x} - \mathbf{x}_n) = \nabla \sum_{n=1}^N \phi_n W_{\sigma_0}(\mathbf{x} - \mathbf{x}_n) \quad (5.13)$$

for some interpolation function  $W_{\sigma_0}$ . This condition was already discovered in [8], and reflects the essential property of the Whitney forms [36] described in Eq. (4.7). Here, the discussion of this condition merely contributes that, in a Hamiltonian context, the motivation for the constraint in Eq. (5.13) is the canonicity of the group action.

With the canonical group action of Eq. (5.7) action in hand, its associated momentum map  $\mu_d$  (equivalently,  $J_d$ ) on  $M_d$  can be sought, using the symplectic structure of Eq. (5.4). First, the infinitesimal generator  $\phi_{M_d}$  of the group action on  $M_d$  must be found, as analogously defined in Eq. (3.51). Given the group action of Eq. (5.7),  $\phi_{M_d}$  takes the form (already implicitly used in Eq. (5.11))

$$\{\{\cdot, J_d(\phi)\}\}_d = - \sum_{i=1}^L \nabla_d^+ \phi(\mathbf{X}_i) \cdot \frac{\partial}{\partial \mathbf{P}_i} - \sum_{n=1}^N (\nabla_d^+ \phi)_n \cdot \frac{\partial}{\partial \mathbf{A}_n}, \quad (5.14)$$

where the pairing of the momentum map with  $\phi$  is denoted  $\langle \mu_d, \phi \rangle = J_d(\phi)$ . The

Poisson bracket of Eq. (5.4) therefore requires that  $J_d(\phi)$  be given by

$$\begin{aligned} J_d(\phi) &= \sum_{n=1}^N (\nabla_d^+ \phi)_n \cdot \left[ \sum_{i=1}^L \int_{-\infty}^{\mathbf{X}_i} d\mathbf{X}'_i W_{\sigma_1}(\mathbf{X}'_i - \mathbf{x}_n) - \mathbf{Y}_n \right] \\ &= \sum_{n=1}^N \phi_n \nabla_d^- \cdot \left[ - \sum_{i=1}^L \int_{-\infty}^{\mathbf{X}_i} d\mathbf{X}'_i W_{\sigma_1}(\mathbf{X}'_i - \mathbf{x}_n) + \mathbf{Y}_n \right] \end{aligned} \quad (5.15)$$

where in the second line has been ‘summed by parts’ [40] using the discrete divergence operator

$$\nabla_d^\pm \cdot \mathbf{v}_n := \pm \sum_{\alpha=1}^3 \frac{v_{n\pm\hat{\alpha}}^\alpha - v_n^\alpha}{\Delta x^\alpha}. \quad (5.16)$$

Note that  $d\mathbf{X}'_i$  is treated in Eq. (5.15) and hereafter as a vector, with each component integrated individually. Also observe that  $\nabla_d^\pm \cdot \nabla_d^\pm \times = 0$  as an operator (when  $\pm$  signs agree).

Given the pairing defined in Eq. (5.10), the momentum map  $\mu_d$  must therefore be

$$\begin{aligned} (\mu_d(m))_n &= -\nabla_d^- \cdot \sum_{i=1}^L \int_{-\infty}^{\mathbf{X}_i} d\mathbf{X}'_i W_{\sigma_1}(\mathbf{X}'_i - \mathbf{x}_n) + \nabla_d^- \cdot \mathbf{Y}_n \\ &= \rho_n + \nabla_d^- \cdot \mathbf{Y}_n \end{aligned} \quad (5.17)$$

defined at each lattice site  $n \in [1, N]$ . Due to the gauge invariance of  $H_d$  in Eq. (5.5)—that is,  $\Phi_f^* H_d = H_d$ —the full system evolved in *continuous* time by  $H_d$  obeys the conservation law

$$\dot{\mu}_d = 0, \quad (5.18)$$

as in the continuous Vlasov-Maxwell system of Section 3.1.5. Eqs. (5.17)-(5.18) define the conservation law of this discrete Hamiltonian system in continuous time,

systematically derived via the momentum map.

Following the analysis of Eqs. (3.58)-(3.59), this conservation law may be reexpressed by deriving the continuous-time equations of motion of the full Hamiltonian  $H_d$ , as follows:

$$\begin{aligned}
\dot{\mathbf{X}}_i &= \{\{\mathbf{X}_i, H_d\}\}_d = \mathbf{P}_i - \sum_{m=1}^N \mathbf{A}_m W_{\sigma_1}(\mathbf{X}_i - \mathbf{x}_m) \\
\dot{\mathbf{P}}_i &= \{\{\mathbf{P}_i, H_d\}\}_d = \sum_{m=1}^N \left( \dot{\mathbf{X}}_i \cdot \mathbf{A}_m \right) \nabla W_{\sigma_1}(\mathbf{X}_i - \mathbf{x}_m) \\
\dot{\mathbf{A}}_n &= \{\{\mathbf{A}_n, H_d\}\}_d = \mathbf{Y}_n \\
\dot{\mathbf{Y}}_n &= \{\{\mathbf{Y}_n, H_d\}\}_d = \sum_{i=1}^L \dot{\mathbf{X}}_i W_{\sigma_1}(\mathbf{X}_i - \mathbf{x}_n) - (\nabla_d^- \times \nabla_d^+ \times \mathbf{A})_n.
\end{aligned} \tag{5.19}$$

Now substituting  $\dot{\mathbf{Y}}_n$  into the charge conservation law Eqs. (5.17)-(5.18), it is found that

$$0 = \dot{\rho}_n + \nabla_d^- \cdot \mathbf{J}_n \tag{5.20}$$

where

$$\begin{aligned}
\rho_n &:= -\nabla_d^- \cdot \sum_{i=1}^L \int_{-\infty}^{\mathbf{X}_i} d\mathbf{X}'_i W_{\sigma_1}(\mathbf{X}'_i - \mathbf{x}_n) \\
\mathbf{J}_n &:= \sum_{i=1}^L \dot{\mathbf{X}}_i W_{\sigma_1}(\mathbf{X}_i - \mathbf{x}_n).
\end{aligned} \tag{5.21}$$

This is an alternative form of the charge conservation law Eq. (5.18) for the continuous-time evolution of this discrete Hamiltonian system.

The form of  $\rho_n$  in Eq. (5.21) can be justified by a schematic one-dimensional example in which  $W_{\sigma_1}(x) = 1$  on  $0 \leq x < \Delta x$  and 0 otherwise. For a single particle

at  $X_i = 0.2$ , then,

$$\rho_n = -\nabla_d^- \cdot \int_{-\infty}^{0.2} dX'_i W_{\sigma_1}(X'_i - x_n) = \begin{cases} 0.8/\Delta x & n = 0 \\ 0.2/\Delta x & n = 1 \\ 0 & n \neq 0, 1. \end{cases} \quad (5.22)$$

This result demonstrates the appropriateness of the momentum map's systematically derived charge density.

### 5.2.3 Defining a gauge-compatible splitting for evolution in discrete time

An algorithmic solution of this Hamiltonian system can now be defined via a gauge-compatible splitting method, whose preservation of  $\mu_d$  will be demonstrated. To algorithmically evolve this system in discrete time, a splitting method is adapted from [9, 12]. In particular, the following Hamiltonian subsystems of Eq. (5.5) can be defined:

$$H_d = \sum_{\alpha=1}^3 H_{\text{Klim}}^\alpha + H_{\mathbf{A}} + H_{\mathbf{Y}} \quad (5.23)$$

where

$$\begin{aligned} H_{\text{Klim}}^\alpha &:= \frac{1}{2} \sum_{i=1}^L \left( P_i^\alpha - A^\alpha(\mathbf{X}_i) \right)^2 \\ H_{\mathbf{A}} &:= \frac{1}{2} \sum_{n=1}^N \left| \nabla_d^+ \times \mathbf{A} \right|_n^2 \\ H_{\mathbf{Y}} &:= \frac{1}{2} \sum_{n=1}^N \mathbf{Y}_n^2. \end{aligned} \quad (5.24)$$

It can be immediately seen that these subsystems are all gauge invariant for the group action of Eq. (5.7)— $\Phi_f^* H_i = H_i \forall f \in \mathcal{F}_d$  and  $i$ . Therefore, if they can be exactly solved, they will comprise a gauge-compatible splitting and preserve  $\mu_d$ .

The equations of motion for each subsystem  $H_i$  may be examined in turn. Applying the canonical Poisson bracket of Eq. (5.4) to each  $H_i$  yields:

$$H_{\text{Klim}}^\alpha \left\{ \begin{array}{l} \dot{X}_i^\beta = \delta_\alpha^\beta \left[ P_i^\alpha - \sum_{m=1}^N A_m^\alpha W_{\sigma_1}(\mathbf{X}_i - \mathbf{x}_m) \right] \\ \dot{P}_i^\beta = \dot{X}_i^\alpha \sum_{m=1}^N A_m^\alpha \partial_\beta W_{\sigma_1}(\mathbf{X}_i - \mathbf{x}_m) \\ \dot{A}_n^\beta = 0 \\ \dot{Y}_n^\beta = \delta_\alpha^\beta \sum_{i=1}^L \dot{X}_i^\alpha W_{\sigma_1}(\mathbf{X}_i - \mathbf{x}_n) \end{array} \right. \quad (5.25)$$

$$H_{\mathbf{A}} \left\{ \begin{array}{l} \dot{\mathbf{X}}_i = 0 \\ \dot{\mathbf{P}}_i = 0 \\ \dot{\mathbf{A}}_n = 0 \\ \dot{\mathbf{Y}}_n = -(\nabla_d^- \times \nabla_d^+ \times \mathbf{A})_n \end{array} \right. \quad (5.26)$$

and

$$H_{\mathbf{Y}} \left\{ \begin{array}{l} \dot{\mathbf{X}}_i = 0 \\ \dot{\mathbf{P}}_i = 0 \\ \dot{\mathbf{A}}_n = \mathbf{Y}_n \\ \dot{\mathbf{Y}}_n = 0 \end{array} \right. \quad (5.27)$$

where  $\partial_\beta \equiv \partial/\partial X_i^\beta$ . (Note that  $\alpha$  is fixed, and is not summed over in the expressions for  $H_{\text{Klim}}^\alpha$ .)  $H_{\mathbf{A}}$  and  $H_{\mathbf{Y}}$  are exactly solvable at a glance. Furthermore,  $H_{\text{Klim}}^\alpha$  is seen

to be exactly solvable by noting that  $\dot{X}_i^\beta = 0$ ;  $\dot{X}_i^\beta$  is therefore a constant determined by a time step's initial conditions. The evolutions of  $\dot{\mathbf{P}}_i$  and  $\dot{\mathbf{Y}}_n$  in  $H_{\text{Klim}}^\alpha$  follow immediately from this analysis.

The exact time evolutions of  $H_{\mathbf{A}}$ ,  $H_{\mathbf{Y}}$  and  $H_{\text{Klim}}^\alpha$  are therefore explicitly solved, defining by construction an explicit-time-advance gauge-compatible splitting method that exactly preserves the momentum map,  $\mu_d = 0$ , as desired. Note that the alternative form of the charge conservation law given in Eq. (5.20)—that is,  $\dot{\rho}_n + \nabla_d^- \cdot \mathbf{J}_n = 0$ —is also exactly preserved in this algorithm, because the substitution that led from Eq. (5.18) to Eq. (5.20)—that is,  $\nabla_d^- \cdot \dot{\mathbf{Y}}_n = \nabla_d^- \cdot \mathbf{J}_n$ —holds for each Hamiltonian subsystem above.

Finally, note that the momentum map  $\mu_d$  has significant ramifications for the appropriate initial conditions of the preceding algorithm. A brief but important discussion of these initial conditions appears in the text following Eq. (5.30) below, and their usefulness in a numerical demonstration will appear in Section 5.3.

### 5.2.4 Symplectic reduction of the method

The symplectic reduction of the previous section's Vlasov-Maxwell Poisson structure is now examined. Since symplectic reduction preserves the momentum map, it is to be expected that the gauge structure of the previous section's GCSM will be preserved in the discrete-time evolution of the reduced equations of motion (as indeed it will). The resulting PIC method recovers that of Xiao *et al.* [8], which employs the splitting method of He *et al.* [9] for the reduced Vlasov-Maxwell bracket of Eq. (3.62).

This PIC scheme will be derived by undertaking the symplectic reduction [57] of the discrete canonical bracket defined in Eq. (5.4). As in Section 3.1.5, a mapping to the reduced symplectic manifold  $\tilde{M}_{d0} = \mu_d^{-1}(0)/\mathcal{F}_d$  is defined, with coordinates given

by

$$\begin{aligned} \pi_{d,\text{red}} : \quad & \mu_d^{-1}(0) \subset M_d \quad \longrightarrow \quad \tilde{M}_{d0} = \mu_d^{-1}(0)/\mathcal{F}_d \\ & (\mathbf{X}_i, \mathbf{P}_i, \mathbf{A}_n, \mathbf{Y}_n) \quad \longmapsto \quad (\mathbf{X}_i, \mathbf{V}_i, \mathbf{B}_n, \mathbf{E}_n), \end{aligned} \quad (5.28)$$

where

$$\begin{aligned} \mathbf{X}_i &= \mathbf{X}_i \\ \mathbf{V}_i &= \mathbf{P}_i - \mathbf{A}(\mathbf{X}_i) \\ \mathbf{B}_n &= (\nabla_d^+ \times \mathbf{A})_n \\ \mathbf{E}_n &= -\mathbf{Y}_n. \end{aligned} \quad (5.29)$$

As discussed earlier, care must be taken to ensure that the discrete fields  $\mathbf{B}_n$  and  $\mathbf{E}_n$  of  $\tilde{M}_{d0}$  obey the reduced manifold constraints

$$\begin{aligned} (\nabla_d^+ \cdot \mathbf{B})_n &= 0 \\ -\nabla_d^- \cdot \sum_{i=1}^L \int_{-\infty}^{\mathbf{X}_i} d\mathbf{X}'_i W_{\sigma_1}(\mathbf{X}'_i - \mathbf{x}_n) - (\nabla_d^- \cdot \mathbf{E})_n &= 0. \end{aligned} \quad (5.30)$$

These constraints must also be satisfied by any initial condition of the algorithm. The former condition is necessary to enforce a physically valid magnetic field. If the latter condition (Gauss's law) is not satisfied initially, it will have the effect of adding fixed 'external' charges at the corresponding vertex  $n$ . In particular, a non-zero initial Gauss's law condition will evolve the system along some other reduced manifold  $\tilde{M}_{d\alpha} = \mu_d^{-1}(\alpha)/\mathcal{F}_d$  with fixed external charge density  $\alpha$ .

A similar initial condition must be determined for the unreduced algorithm of Section 5.2.1 as well. The unreduced algorithm enforces the constraint  $(\nabla_d^+ \cdot \nabla_d^+ \times \mathbf{A})_n = 0$  automatically. However, for simulations without external charges, care should be taken so that the value of  $(\mu_d(m))_n$  in Eq. (5.17) is every-

where initialized to zero. (Alternatively, Eq. (5.17) can be used to properly initialize a simulation with external charges that remain fixed for all time, as will be used to advantage in numerical examples of Section 5.3.) Note that the derivation of the momentum map is essential to this correct specification of initial conditions.

The reduction of the discrete system may therefore proceed, and Eq. (5.29) can be substituted into the bracket of Eq. (5.4) to find

$$\begin{aligned}
\{\{F, G\}\}_d^{\text{red}}[\mathbf{X}_i, \mathbf{V}_i, \mathbf{B}_n, \mathbf{E}_n] = & \\
& \sum_{i=1}^L \left( \frac{\partial F}{\partial \mathbf{X}_i} \cdot \frac{\partial G}{\partial \mathbf{V}_i} - \frac{\partial G}{\partial \mathbf{X}_i} \cdot \frac{\partial F}{\partial \mathbf{V}_i} + \left[ \frac{\partial F}{\partial \mathbf{V}_i} \times \frac{\partial G}{\partial \mathbf{V}_i} \right] \cdot \sum_{n=1}^N \mathbf{B}_n W_{\sigma_2}(\mathbf{X}_i - \mathbf{x}_n) \right) \\
& + \sum_{n=1}^N \left( \left[ \sum_{i=1}^L \frac{\partial F}{\partial \mathbf{V}_i} W_{\sigma_1}(\mathbf{X}_i - \mathbf{x}_n) - \left( \nabla_d^- \times \frac{\partial F}{\partial \mathbf{B}} \right)_n \right] \cdot \frac{\partial G}{\partial \mathbf{E}_n} \right. \\
& \quad \left. - \left[ \sum_{i=1}^L \frac{\partial G}{\partial \mathbf{V}_i} W_{\sigma_1}(\mathbf{X}_i - \mathbf{x}_n) - \left( \nabla_d^- \times \frac{\partial G}{\partial \mathbf{B}} \right)_n \right] \cdot \frac{\partial F}{\partial \mathbf{E}_n} \right).
\end{aligned} \tag{5.31}$$

To derive the  $\partial_{\mathbf{V}_i} F \times \partial_{\mathbf{V}_i} G \cdot \mathbf{B}(\mathbf{X}_i)$  term in the bracket above, the interpolation functions were required to satisfy an additional constraint

$$\nabla \times \sum_{n=1}^N \mathbf{A}_n W_{\sigma_1}(\mathbf{x} - \mathbf{x}_n) = \sum_{n=1}^N (\nabla_d^+ \times \mathbf{A})_n W_{\sigma_2}(\mathbf{x} - \mathbf{x}_n) \tag{5.32}$$

for some interpolation function  $W_{\sigma_2}$ . As in Eq. (5.13), this is another appearance (for a higher-degree form) of the Whitney interpolant constraint.

Lastly, the Hamiltonian in the reduced coordinates of  $\tilde{M}_{d0}$  can be reexpressed as

$$H_d^{\text{red}}[\mathbf{X}_i, \mathbf{V}_i, \mathbf{B}_n, \mathbf{E}_n] = \frac{1}{2} \sum_{i=1}^L \mathbf{V}_i^2 + \frac{1}{2} \sum_{n=1}^N \left( \mathbf{E}_n^2 + \mathbf{B}_n^2 \right). \tag{5.33}$$

Thus the reduced Hamiltonian system of Xiao *et al.* [8] has been recovered.

As discussed in Section 3.1.5 for spatially continuous systems, this reduced Hamil-

tonian system is automatically guaranteed to preserve the momentum map of its parent, so long as its evolution is constrained to  $\tilde{M}_{d0}$ . To see that this is the case, its evolution equations may be computed under the splitting scheme analogous to the unreduced case, defined by [8, 9, 12]

$$H_d^{\text{red}} = \sum_{\alpha=1}^3 H_{\mathbf{V}}^{\alpha} + H_{\mathbf{B}} + H_{\mathbf{E}} \quad (5.34)$$

where

$$\begin{aligned} H_{\mathbf{V}}^{\alpha} &:= \frac{1}{2} \sum_{i=1}^L (V_i^{\alpha})^2 \\ H_{\mathbf{B}} &:= \frac{1}{2} \sum_{n=1}^N \mathbf{B}_n^2 \\ H_{\mathbf{E}} &:= \frac{1}{2} \sum_{n=1}^N \mathbf{E}_n^2. \end{aligned} \quad (5.35)$$

These subsystems generate the following equations of motion:

$$H_{\mathbf{V}}^{\alpha} \left\{ \begin{aligned} \dot{X}_i^{\beta} &= \delta_{\alpha}^{\beta} V_i^{\alpha} \\ \dot{V}_i^{\beta} &= \epsilon_{\beta\alpha\gamma} V_i^{\alpha} \sum_{n=1}^N B_n^{\gamma} W_{\sigma_2}(\mathbf{X}_i - \mathbf{x}_n) \\ \dot{B}_n^{\beta} &= 0 \\ \dot{E}_n^{\beta} &= -\delta_{\alpha}^{\beta} \sum_{i=1}^L V_i^{\alpha} W_{\sigma_1}(\mathbf{X}_i - \mathbf{x}_n) \end{aligned} \right. \quad (5.36)$$

$$H_{\mathbf{B}} \left\{ \begin{aligned} \dot{\mathbf{X}}_i &= 0 \\ \dot{\mathbf{V}}_i &= 0 \\ \dot{\mathbf{B}}_n &= 0 \\ \dot{\mathbf{E}}_n &= (\nabla_d^- \times \mathbf{B})_n \end{aligned} \right. \quad (5.37)$$

$$H_{\mathbf{E}} \begin{cases} \dot{\mathbf{X}}_i &= 0 \\ \dot{\mathbf{V}}_i &= \sum_{n=1}^N \mathbf{E}_n W_{\sigma_1}(\mathbf{X}_i - \mathbf{x}_n) \\ \dot{\mathbf{B}}_n &= -(\nabla_d^+ \times \mathbf{E})_n \\ \dot{\mathbf{E}}_n &= 0. \end{cases} \quad (5.38)$$

Note again that  $\alpha$  is not summed over in the expressions for subsystem  $H_{\mathbb{V}}^\alpha$ .

Upon inspection, it is evident that the  $\tilde{M}_{d0}$  constraints of Eq. (5.30) are obeyed in each subsystem when they are exactly solved. (As in the unreduced case, the above subsystems are readily exactly solved. In particular, note that  $\dot{V}_i^\alpha = 0$  in  $H_{\mathbb{V}}^\alpha$ .) Consequently, the exact conservation law of the reduced system is systematically derived by simply expressing the unreduced momentum map of Eq. (5.17) in  $\tilde{M}_{d0}$  coordinates

$$\begin{aligned} (\bar{\mu}_d)_n &= -\nabla_d^- \cdot \sum_{i=1}^L \int_{-\infty}^{\mathbf{X}_i} d\mathbf{X}'_i W_{\sigma_1}(\mathbf{X}'_i - \mathbf{x}_n) - \nabla_d^- \cdot \mathbf{E}_n \\ &:= \rho_n - \nabla_d^- \cdot \mathbf{E}_n \\ &= 0, \end{aligned} \quad (5.39)$$

where in the final line it has been noted that  $\bar{\mu}_d$  vanishes by the previous choice of reduction to the preimage of zero under  $\mu_d$ —the submanifold  $\mu_d^{-1}(0)$ . Eq. (5.39) is Gauss's law, which is by construction guaranteed to be preserved,

$$\dot{\bar{\mu}}_d = 0, \quad (5.40)$$

as desired. (An analogous conservation law was found for the reduced bracket in the FEEC formalism of Kraus *et al.* [15], where the momentum map was treated as a Casimir.) The local charge conservation law of Eq. (5.20)—whose ex-

pression is unmodified in the reduced submanifold—is furthermore satisfied, since  $\nabla_d^- \cdot \dot{\mathbf{E}}_n = -\nabla_d^- \cdot \mathbf{J}_n$  holds in each subsystem of  $H_d^{\text{red}}$ .

## 5.3 A GCSM for PIC simulations using FEEC and its numerical implementation

A second canonical Poisson structure and Hamiltonian is now defined for the Vlasov-Maxwell system—this time, discretized using the techniques of finite element exterior calculus [15, 34, 35]. This discussion will emphasize the role of the momentum map in enabling the precise assignment of a fixed, non-dynamical background charge density. Numerical results will be presented for Landau damping and Weibel instability simulations. The following calculations are performed in Gaussian units.

### 5.3.1 The finite element electromagnetic Poisson structure

To begin, consider electromagnetic fields over a continuous manifold  $\Omega \subset \mathbb{R}^3$  in the temporal gauge. The configuration space for such fields is the set  $Q = \{\mathbf{A} \mid \mathbf{A} \in \Lambda^1(\Omega)\}$  of possible vector potentials, defined as differential 1-forms over  $\Omega$ . To find a variable conjugate to  $\mathbf{A}(\mathbf{x})$ , the following variational derivative of the electromagnetic Lagrangian may be computed,

$$L_{\text{EM}} = \frac{1}{8\pi} \int d\mathbf{x} \left( \left| -\frac{1}{c} \dot{\mathbf{A}} \right|^2 - |d\mathbf{A}|^2 \right), \quad \mathbf{Y} = \frac{\delta L_{\text{EM}}}{\delta \dot{\mathbf{A}}} = \frac{\dot{\mathbf{A}}}{4\pi c^2}. \quad (5.41)$$

Clearly,  $\mathbf{Y} \in \Lambda^1(\Omega)$  is also a 1-form over  $\Omega$  corresponding to negative the electric field,  $\mathbf{Y} = -\mathbf{E}/4\pi c$ . As in Eq. (4.16),  $|\alpha|^2 = (\alpha, \alpha)_p$  in Eq. (5.41) denotes the standard inner product on  $\mathbb{R}^3$  for  $p = 1, 2$ .

The full phase space is then given by the cotangent bundle  $T^*Q = \{\mathbf{A}, \mathbf{Y}\}$  with

canonical symplectic structure defined by the Poisson bracket [59]

$$\{F, G\} = \int \left( \frac{\delta F}{\delta \mathbf{A}} \cdot \frac{\delta G}{\delta \mathbf{Y}} - \frac{\delta G}{\delta \mathbf{A}} \cdot \frac{\delta F}{\delta \mathbf{Y}} \right) d\mathbf{x} \quad (5.42)$$

(as in Eq. 3.39). Here,  $F[\mathbf{A}, \mathbf{Y}]$  and  $G[\mathbf{A}, \mathbf{Y}]$  are arbitrary functionals on  $T^*Q$ .

This geometric description of fields on  $\Omega$  is now mapped to its triangulation  $\mathcal{T}_h$ . On  $\mathcal{T}_h$ , the fields  $\mathbf{A}$  and  $\mathbf{Y}$  can be defined by their expansion in the corresponding basis for finite element 1-forms:

$$\begin{aligned} \mathbf{A}(t, \mathbf{x}) &= \mathbf{a}(t) \cdot \boldsymbol{\Lambda}^1(\mathbf{x}) \\ \mathbf{Y}(t, \mathbf{x}) &= \mathbf{y}(t) \cdot \mathbb{M}_1^{-1} \cdot \boldsymbol{\Lambda}^1(\mathbf{x}). \end{aligned} \quad (5.43)$$

Here,  $\boldsymbol{\Lambda}^1$  is an  $N_1 \times 1$  vector of basis elements and  $\mathbf{a}, \mathbf{y} \in \mathbb{R}^{N_1}$  denote coefficients, as in Eq. (4.12).  $\mathbf{a}$  and  $\mathbf{y}$  are identified as dynamical variables by explicitly notating their time dependence. The inverse factor of the 1-form mass matrix  $\mathbb{M}_1$  in Eq. (5.43) follows from computing the conjugate momentum of  $\mathbf{a}$  in the following discretization of  $L_{\text{EM}}$ :

$$\begin{aligned} L_{\text{EM}} &= \frac{1}{8\pi} \int_{|\mathcal{T}_h|} d\mathbf{x} \left( \left| -\frac{1}{c} \dot{\mathbf{a}} \cdot \boldsymbol{\Lambda}^1 \right|^2 - |\mathbf{a} \cdot d\boldsymbol{\Lambda}^1|^2 \right) \\ &= \frac{1}{8\pi} \int_{|\mathcal{T}_h|} d\mathbf{x} \left( \frac{1}{c^2} \dot{\mathbf{a}} \cdot \mathbb{M}_1 \cdot \dot{\mathbf{a}} - \mathbf{a} \cdot \mathbb{C}^T \mathbb{M}_2 \mathbb{C} \cdot \mathbf{a} \right), \quad \mathbf{y} = \frac{\delta L_{\text{EM}}}{\delta \dot{\mathbf{a}}} = \frac{\mathbb{M}_1 \dot{\mathbf{a}}}{4\pi c^2} \end{aligned} \quad (5.44)$$

where  $d\boldsymbol{\Lambda}^1 = \mathbb{C}^T \boldsymbol{\Lambda}^2$  has been substituted from Table 4.1 and mass matrices were applied as defined in Eq. (4.15). Comparing Eqs. (5.41) and Eq. (5.44) yields the desired expansion for  $\mathbf{Y}$  in Eq. (5.43). The inverse factor of  $\mathbb{M}_1$  will also be seen to ensure that the Poisson bracket of Eq. (5.49) is canonical.

To discretize the Poisson bracket of Eq. (5.42), one would first like to express  $\delta F/\delta \mathbf{A}$  for a discrete variation  $\delta \mathbf{A} = \delta \mathbf{a} \cdot \boldsymbol{\Lambda}^1$  in terms of  $\partial F/\partial \mathbf{a}$ . Since variational derivatives are valued dually to their variations, following [15] it is appropriate to

require that

$$\left\langle \frac{\delta F}{\delta \mathbf{A}}, \delta \mathbf{a} \cdot \boldsymbol{\Lambda}^1 \right\rangle_{L^2 \Lambda^1} = \left\langle \frac{\partial F}{\partial \mathbf{a}}, \delta \mathbf{a} \right\rangle_{\mathbb{R}^{N_1}}. \quad (5.45)$$

Here,  $\langle \cdot, \cdot \rangle_{L^2 \Lambda^1} = \int_{|\mathcal{T}_h|} d\mathbf{x} (\cdot, \cdot)_{p=1}$  denotes the  $L^2 \Lambda^1$  inner product, and  $\langle \cdot, \cdot \rangle_{\mathbb{R}^{N_1}}$  the standard inner product on  $\mathbb{R}^{N_1}$ . In particular, setting  $\delta a_j = \delta_{ij}$  for some fixed, arbitrary  $i \in [1, N_1]$  and using  $(\cdot, \cdot)_p$  as defined in Eq. (4.16), Eq. (5.45) yields

$$\int_{|\mathcal{T}_h|} d\mathbf{x} \left( \frac{\delta F}{\delta \mathbf{A}}, \Lambda_i^1(\mathbf{x}) \right)_{p=1} = \frac{\partial F}{\partial a_i}. \quad (5.46)$$

Eq. (5.46) may be solved for  $\delta F / \delta \mathbf{A}$  by expanding it in the  $\boldsymbol{\Lambda}^1$  basis, setting  $\delta F / \delta \mathbf{A} = \mathbf{f} \cdot \boldsymbol{\Lambda}^1$  for some  $\mathbf{f} \in \mathbb{R}^{N_1}$ . Using the 1-form mass matrix  $\mathbb{M}_1$  from Eq. (4.15), Eq. (5.46) is found to imply that  $\mathbf{f} = \mathbb{M}_1^{-1} \cdot \partial F / \partial \mathbf{a}$ . Therefore,

$$\frac{\delta F}{\delta \mathbf{A}} = \frac{\partial F}{\partial \mathbf{a}} \cdot \mathbb{M}_1^{-1} \cdot \boldsymbol{\Lambda}^1. \quad (5.47)$$

The discrete variation  $\delta \mathbf{Y} = \delta \mathbf{y} \cdot \mathbb{M}_1^{-1} \cdot \boldsymbol{\Lambda}^1$  establishes a similar result for  $\mathbf{Y}$ , namely

$$\frac{\delta F}{\delta \mathbf{Y}} = \frac{\partial F}{\partial \mathbf{y}} \cdot \boldsymbol{\Lambda}^1. \quad (5.48)$$

Thus, to derive the discrete Poisson bracket, Eqs. (5.47)-(5.48) are substituted into Eq. (5.42), which is integrated over  $|\mathcal{T}_h|$  to find:

$$\{F, G\} = \frac{\partial F}{\partial \mathbf{a}} \cdot \frac{\partial G}{\partial \mathbf{y}} - \frac{\partial G}{\partial \mathbf{a}} \cdot \frac{\partial F}{\partial \mathbf{y}}. \quad (5.49)$$

True to its continuous counterpart in Eq. (5.42), the discrete Poisson bracket of Eq. (5.49) is in canonical (Darboux coordinate) symplectic form.

### 5.3.2 The finite element Vlasov-Maxwell system

The full Poisson structure of the discrete Vlasov-Maxwell system readily follows from the the foregoing analysis of its electromagnetic subsystem. To describe a system of  $L$  particles, let  $\mathbf{X}_\ell, \mathbf{P}_\ell \in \mathbb{R}^3$   $\ell \in [1, L]$  denote the position and momentum of the  $\ell^{\text{th}}$  particle and let  $m_\ell$  and  $q_\ell$  denote its mass and charge. Particles may then be characterized by a Klimontovich distribution,  $f(\mathbf{x}, \mathbf{p}) = \sum_\ell \delta(\mathbf{x} - \mathbf{X}_\ell) \delta(\mathbf{p} - \mathbf{P}_\ell)$ . Particle phase space is defined as usual with a canonical bracket on position  $\mathbf{X}_\ell$  and momentum  $\mathbf{P}_\ell$ .

Combining Eq. (5.49) with the Poisson bracket for these  $L$  particles, therefore, the discrete Vlasov-Maxwell Poisson structure is given by

$$\{F, G\} = \frac{\partial F}{\partial \mathbf{a}} \cdot \frac{\partial G}{\partial \mathbf{y}} - \frac{\partial G}{\partial \mathbf{a}} \cdot \frac{\partial F}{\partial \mathbf{y}} + \sum_{\ell=1}^L \left( \frac{\partial F}{\partial \mathbf{X}_\ell} \cdot \frac{\partial G}{\partial \mathbf{P}_\ell} - \frac{\partial G}{\partial \mathbf{X}_\ell} \cdot \frac{\partial F}{\partial \mathbf{P}_\ell} \right). \quad (5.50)$$

Here,  $F$  and  $G$  are arbitrary functionals on the discrete Poisson manifold  $(M_d, \{\cdot, \cdot\})$ , where each point  $m_d \in M_d$  is defined by the data

$$\begin{aligned} m_d &= (\mathbf{a}, \mathbf{y}, \mathbf{X}_1, \dots, \mathbf{X}_L, \mathbf{P}_1, \dots, \mathbf{P}_L) \\ &\in \mathbb{R}^{N_1} \times \mathbb{R}^{N_1} \times \mathbb{R}^{3L} \times \mathbb{R}^{3L}. \end{aligned} \quad (5.51)$$

A Hamiltonian  $H_{\text{VM}} = H_{\text{VM}}[\mathbf{a}, \mathbf{y}, \mathbf{X}_i, \mathbf{P}_i]$  can now be defined on  $M_d$ , given in Gaussian units by

$$\begin{aligned} H_{\text{VM}} &= H_{\text{EM}} + H_{\text{Kinetic}} \\ \text{where } H_{\text{EM}} &= \frac{1}{8\pi} \int_{|\mathcal{T}_h|} d\mathbf{x} (|-4\pi c \mathbf{Y}|^2 + |d\mathbf{A}|^2) \\ &= \frac{1}{8\pi} \left( (4\pi c)^2 \mathbf{y} \cdot \mathbf{M}_1^{-1} \cdot \mathbf{y} + \mathbf{a} \cdot \mathbf{C}^T \mathbf{M}_2 \mathbf{C} \cdot \mathbf{a} \right) \\ H_{\text{Kinetic}} &= \sum_{\ell=1}^L \frac{1}{2m_\ell} \left| \mathbf{P}_\ell - \frac{q_\ell}{c} \mathbf{A}(\mathbf{X}_\ell) \right|^2, \end{aligned} \quad (5.52)$$

where  $\mathbf{A}(\mathbf{X}_\ell) = \mathbf{a} \cdot \boldsymbol{\Lambda}^1(\mathbf{X}_\ell)$ . In  $H_{\text{EM}}$ , Eqs. (4.15) and (5.43) have been substituted and  $\mathbb{C}^T \boldsymbol{\Lambda}^2 = d\boldsymbol{\Lambda}^1$  from Table 4.1 was used. The difference in  $H_{\text{Kinetic}}$  is taken componentwise, i.e.  $P_{\ell\mu} - (q_\ell/c)\mathbf{a} \cdot \boldsymbol{\Lambda}^1(\mathbf{X}_\ell)_\mu$  for  $\mu \in \{1, 2, 3\}$ . Hereafter, components of  $\mathbf{P}_\ell$  will be denoted by  $P_{\ell\mu}$  and those of  $\mathbf{X}_\ell$  by  $X_\ell^\mu$ .

### 5.3.3 Gauge structure

The gauge structure of this discrete Vlasov-Maxwell system is now examined and its corresponding momentum map is derived. First note that because  $\mathbb{C}\mathbb{G} = 0$ ,  $H_{\text{VM}}$  of Eq. (5.52) is invariant under any gauge transformation  $\Phi_{\text{exp}(\mathbf{s})} : M_d \rightarrow M_d$  of the form

$$\Phi_{\text{exp}(\mathbf{s})} \begin{pmatrix} \mathbf{a} \\ \mathbf{y} \\ \mathbf{X}_\ell \\ \mathbf{P}_\ell \end{pmatrix} = \begin{pmatrix} \mathbf{a} + \mathbb{G}\mathbf{s} \\ \mathbf{y} \\ \mathbf{X}_\ell \\ \mathbf{P}_\ell + \frac{q_\ell}{c}\mathbb{G}\mathbf{s} \cdot \boldsymbol{\Lambda}^1(\mathbf{X}_\ell) \end{pmatrix} \quad (5.53)$$

$\forall \ell \in [1, L], \mathbf{s} \in \mathbb{R}^{N_0}$ . Since  $\Phi_{\text{exp}(\mathbf{s})} \circ \Phi_{\text{exp}(\mathbf{t})} = \Phi_{\text{exp}(\mathbf{s}+\mathbf{t})}$ , such transformations form an abelian group. Evidently, they are also generated by vector fields  $X_{\mathbf{s}} \in \mathfrak{X}(M_d)$  of the form

$$X_{\mathbf{s}} = \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} \Phi_{\text{exp}(\epsilon\mathbf{s})} = \mathbb{G}_{jk} s_k \left[ \partial_{a_j} + \sum_{\ell=1}^L \frac{q_\ell}{c} \Lambda_j^1(\mathbf{X}_\ell)_\mu \partial_{P_{\ell\mu}} \right] \quad (5.54)$$

expressed using Einstein summation convention.

It can again be checked whether  $\Phi$  of Eq. (5.53) is a canonical transformation, that is, whether it preserves the Poisson bracket of Eq. (5.50)—

$$\{F, G\} \circ \Phi_{\text{exp}(\mathbf{s})} = \{F \circ \Phi_{\text{exp}(\mathbf{s})}, G \circ \Phi_{\text{exp}(\mathbf{s})}\} \quad (5.55)$$

$\forall \mathbf{s}$ . Infinitesimally, it is examined whether

$$X_{\mathbf{s}}(\{F, G\}) = \{X_{\mathbf{s}}(F), G\} + \{F, X_{\mathbf{s}}(G)\}. \quad (5.56)$$

After canceling terms by the equality of mixed partials, verifying Eq. (5.56) reduces to checking that

$$\begin{aligned} 0 &= \sum_{\ell=1}^L \frac{q_{\ell}}{c} \mathbb{G}_{jk} s_k \left[ \partial_{X_{\ell}^{\nu}} \Lambda_j^1(\mathbf{X}_{\ell})_{\mu} - \partial_{X_{\ell}^{\mu}} \Lambda_j^1(\mathbf{X}_{\ell})_{\nu} \right] (\partial_{P_{\ell\mu}} F) (\partial_{P_{\ell\nu}} G) \\ &= \sum_{\ell=1}^L \frac{q_{\ell}}{c} \left[ \mathbb{G}\mathbf{s} \cdot d\Lambda^1(\mathbf{X}_{\ell})_{\nu\mu} \right] (\partial_{P_{\ell\mu}} F) (\partial_{P_{\ell\nu}} G). \end{aligned} \quad (5.57)$$

Each term in this sum is seen to vanish, however, since

$$\mathbb{G}\mathbf{s} \cdot d\Lambda^1 = \mathbf{s} \cdot \mathbb{G}^T d\Lambda^1 = \mathbf{s} \cdot d(\mathbb{G}^T \Lambda^1) = \mathbf{s} \cdot dd\Lambda^0 = 0. \quad (5.58)$$

Thus,  $X_{\mathbf{s}}$  generates a canonical group action, as desired.

The momentum map  $\mu$  of this canonical group action is found by solving for its generating functions. That is, for any  $\mathbf{s} \in \mathbb{R}^{N_0}$ , a generating function  $\mu_{\mathbf{s}}$  is sought such that  $X_{\mathbf{s}} = \{\cdot, \mu_{\mathbf{s}}\}$  as derivations, as in Eq. (3.14). By comparing Eqs. (5.50) and (5.54),  $X_{\mathbf{s}} = \{\cdot, \mu_{\mathbf{s}}\}$  is found to hold if and only if

$$\begin{aligned} \frac{\partial \mu_{\mathbf{s}}}{\partial \mathbf{a}} &= 0 \\ \frac{\partial \mu_{\mathbf{s}}}{\partial \mathbf{y}} &= \mathbb{G}\mathbf{s} \\ \frac{\partial \mu_{\mathbf{s}}}{\partial \mathbf{X}_{\ell}} &= -\frac{q_{\ell}}{c} \mathbb{G}\mathbf{s} \cdot \Lambda^1(\mathbf{X}_{\ell}) \\ \frac{\partial \mu_{\mathbf{s}}}{\partial \mathbf{P}_{\ell}} &= 0 \quad \forall \ell \in [1, L]. \end{aligned} \quad (5.59)$$

Since  $\mathbb{G}^T \Lambda^1 = d\Lambda^0$  is an exact form, this linear system of partial differential equations

is readily solved by

$$\mu_{\mathbf{s}} = \mathbb{G}\mathbf{s} \cdot \mathbf{y} - \sum_{\ell=1}^L \frac{q_{\ell}}{c} \mathbf{s} \cdot \mathbf{\Lambda}^0(\mathbf{X}_{\ell}). \quad (5.60)$$

The momentum map  $\mu$  characterizing all generating functions  $\{\mu_{\mathbf{s}}\}$  is defined by requiring that  $\mu \cdot \mathbf{s} = \mu_{\mathbf{s}} \forall \mathbf{s}$ . Therefore,  $\mu$  is given by

$$\mu = \mathbb{G}^T \mathbf{y} - \sum_{\ell=1}^L \frac{q_{\ell}}{c} \mathbf{\Lambda}^0(\mathbf{X}_{\ell}). \quad (5.61)$$

Setting  $\mu = 0$ , Eq. (5.61) is a discrete form of Gauss' law,

$$0 = (\nabla \cdot \mathbf{E} - 4\pi\rho)/4\pi c \quad (5.62)$$

where  $\mathbf{E} = -4\pi c \mathbf{Y}$  and  $\rho = \sum_{\ell} q_{\ell} \mathbf{\Lambda}^0(\mathbf{X}_{\ell})$ .

As in Section 5.2, a nonzero value of  $\mu$  indicates that the divergence of the electric field is not entirely accounted for by the dynamical particles labeled  $\ell \in [1, L]$ . Since  $\dot{\mu} = 0$ , the nonzero  $\mu$  acts as a fixed, external, nondynamical background charge that persists throughout a simulation, in a manner that remains entirely structure-preserving. In particular,  $\mu$  may be regarded as representing an external charge density,

$$\mu \sim \rho_{\text{ext}}/c. \quad (5.63)$$

In Section 5.3.6, Eq. (5.63) will be applied to establish precise initial conditions in a PIC simulation.

### 5.3.4 Continuous-time equations of motion

The equations of motion are now derived via the Hamiltonian of Eq. (5.52) and the Poisson bracket of Eq. (5.50). The result is found to be:

$$\begin{aligned}
\dot{X}_\ell^\mu &= \{X_\ell^\mu, H_{\text{VM}}\} = \frac{1}{m_\ell} \left( P_{\ell\mu} - \frac{q_\ell}{c} \mathbf{A}(\mathbf{X}_\ell)_\mu \right) \\
\dot{P}_{\ell\mu} &= \{P_{\ell\mu}, H_{\text{VM}}\} = \frac{q_\ell}{c} \dot{X}_\ell^\nu \partial_{X_\ell^\mu} \mathbf{A}(\mathbf{X}_\ell)_\nu \\
\dot{\mathbf{a}} &= \{\mathbf{a}, H_{\text{VM}}\} = 4\pi c^2 \mathbb{M}_1^{-1} \cdot \mathbf{y} \\
\dot{\mathbf{y}} &= \{\mathbf{y}, H_{\text{VM}}\} = -\frac{1}{4\pi} \mathbb{C}^T \mathbb{M}_2 \mathbb{C} \cdot \mathbf{a} + \sum_{\ell=1}^L \frac{q_\ell}{c} \dot{X}_\ell^\mu \Lambda^1(\mathbf{X}_\ell)_\mu
\end{aligned} \tag{5.64}$$

where  $\mathbf{A}(\mathbf{X}_\ell)_\mu = \mathbf{a} \cdot \Lambda^1(\mathbf{X}_\ell)_\mu$  using the component notation of Eq. (4.13).

As in Section 5.2, these equations of motion allow the reexpression of the momentum map conservation law,  $\dot{\mu} = 0$ , as a discrete, local charge continuity equation in conservative form. In particular, the time derivative  $\dot{\mu}$  of Eq. (5.61) is taken and  $\dot{\mathbf{y}}$  of Eq. (5.64) is substituted, noting  $\mathbb{C}\mathbb{C} = 0$  to find

$$(\mathbb{G}^T \mathbf{j} - \dot{\rho})/c = 0 \tag{5.65}$$

where  $\rho = \sum_\ell q_\ell \Lambda^0(\mathbf{X}_\ell)$  and  $\mathbf{j} = \sum_\ell q_\ell \dot{X}_\ell^\mu \Lambda^1(\mathbf{X}_\ell)_\mu$ . As in Eq. (5.61), a correspondence is noted between the discrete and continuous operators  $\mathbb{G}^T \sim (-\nabla \cdot)$ . Thus, Eq. (5.65) is a discrete equivalent of the charge conservation law  $\partial_t \rho + \nabla \cdot \mathbf{j} = 0$ , as seen in Kraus *et al.* [15].

Eq. (5.64) is sometimes referred to as a semi-discrete system, since it describes a discretely defined system evolving in continuous time. By constructing a gauge-compatible splitting method, the next section now proceeds to a fully discrete algorithm.

### 5.3.5 Discrete-time equations of motion via gauge-compatible splitting

As in Section 5.2, the Vlasov-Maxwell splitting discovered in He *et al.* [9] is adapted to canonical coordinates, and  $H_{\text{VM}}$  is split into five sub-Hamiltonians, as follows:

$$\begin{aligned}
 H_{\text{VM}} &= H_{\mathbf{A}} + H_{\mathbf{Y}} + H_{\text{Kinetic}}^x + H_{\text{Kinetic}}^y + H_{\text{Kinetic}}^z \\
 \text{where} \quad H_{\mathbf{A}} &= \frac{1}{8\pi} \mathbf{a} \cdot \mathbb{C}^T \mathbb{M}_2 \mathbb{C} \cdot \mathbf{a} \\
 H_{\mathbf{Y}} &= \frac{1}{8\pi} (4\pi c)^2 \mathbf{y} \cdot \mathbb{M}_1^{-1} \cdot \mathbf{y} \\
 H_{\text{Kinetic}}^\alpha &= \sum_{\ell=1}^L \frac{1}{2m_\ell} \left( P_{\ell\alpha} - \frac{q_\ell}{c} \mathbf{A}(\mathbf{X}_\ell)_\alpha \right)^2
 \end{aligned} \tag{5.66}$$

$\forall \alpha \in \{x, y, z\}$ . Each sub-Hamiltonian remains invariant under the gauge transformation  $\Phi_{\text{exp(s)}}$  defined in Eq. (5.53).

Repeating the exercise of Eqs. (5.36)-(5.38), the equations of motion of each subsystem are now found, omitting equations for the subsystems' static degrees of freedom:

$$\begin{aligned}
 H_{\mathbf{A}} : \quad \dot{\mathbf{y}} &= -\frac{1}{4\pi} \mathbb{C}^T \mathbb{M}_2 \mathbb{C} \cdot \mathbf{a} \\
 H_{\mathbf{Y}} : \quad \dot{\mathbf{a}} &= 4\pi c^2 \mathbb{M}_1^{-1} \cdot \mathbf{y} \\
 H_{\text{Kinetic}}^\alpha : \quad &\begin{cases} \dot{X}_\ell^\alpha &= \frac{1}{m_\ell} \left( P_{\ell\alpha} - \frac{q_\ell}{c} \mathbf{A}(\mathbf{X}_\ell)_\alpha \right) \\ \dot{P}_{\ell\mu} &= \frac{q_\ell}{c} \dot{X}_\ell^\alpha \partial_{X_\ell^\mu} \mathbf{A}(\mathbf{X}_\ell)_\alpha \\ \dot{\mathbf{y}} &= \sum_{\ell=1}^L \frac{q_\ell}{c} \dot{X}_\ell^\alpha \mathbf{\Lambda}^1(\mathbf{X}_\ell)_\alpha. \end{cases}
 \end{aligned} \tag{5.67}$$

To clarify notation in Eq. (5.67), in the  $H_{\text{Kinetic}}^\alpha$  subsystem,  $\dot{X}_\ell^\mu = 0$  for  $\mu \neq \alpha$ . (Here,  $\alpha$  is regarded as fixed while  $\mu$  ranges over all  $\{x, y, z\}$  indices.) Thus, the equations of motion  $X_\ell^{\mu \neq \alpha}$  are omitted above.

Furthermore, it follows from a simple calculation that  $\ddot{X}_\ell^\alpha = 0$  in  $H_{\text{Kinetic}}^\alpha$  so that

$\dot{X}_\ell^\alpha$  is constant during the evolution of each subsystem. As a result, all subsystems above are exactly integrable. Eq. (5.67) therefore defines a gauge-compatible splitting method.

More concretely, an evolution over the timestep  $[t, t + \Delta]$  in each subsystem is fully specified by

$$\begin{aligned}
H_{\mathbf{A}} : \quad & \mathbf{y}(t + \Delta) = \mathbf{y}(t) - \frac{\Delta}{4\pi} \mathbb{C}^T \mathbb{M}_2 \mathbb{C} \cdot \mathbf{a}(t) \\
H_{\mathbf{Y}} : \quad & \mathbf{a}(t + \Delta) = \mathbf{a}(t) + \Delta 4\pi c^2 \mathbb{M}_1^{-1} \cdot \mathbf{y}(t) \\
H_{\text{Kinetic}}^\alpha : \quad & \\
& \left\{ \begin{aligned}
X_\ell^\alpha(t + \delta) &= X_\ell^\alpha(t) + \frac{\delta}{m_\ell} \left( P_{\ell\alpha}(t) - \frac{q_\ell}{c} \mathbf{a}(t) \cdot \boldsymbol{\Lambda}^1(\mathbf{X}_\ell(t))_\alpha \right) \\
P_{\ell\mu}(t + \Delta) &= P_{\ell\mu}(t) + \frac{q_\ell}{c} \dot{X}_\ell^\alpha(t) \mathbf{a}(t) \cdot \int_t^{t+\Delta} dt' \partial_{X_\ell^\mu(t')} \boldsymbol{\Lambda}^1(\mathbf{X}_\ell(t'))_\alpha \\
\mathbf{y}(t + \Delta) &= \mathbf{y}(t) + \sum_{\ell=1}^L \frac{q_\ell}{c} \dot{X}_\ell^\alpha(t) \int_t^{t+\Delta} dt' \boldsymbol{\Lambda}^1(\mathbf{X}_\ell(t'))_\alpha.
\end{aligned} \right. \quad (5.68)
\end{aligned}$$

In Eq. (5.68),  $t$  is a fixed initial time and  $\delta \in [0, \Delta]$  parametrizes the particle trajectory  $\mathbf{X}_\ell(t) \rightarrow \mathbf{X}_\ell(t + \Delta)$  during one timestep of the  $H_{\text{Kinetic}}^\alpha$  subsystem, which forms a straight line segment in the  $\hat{\alpha}$  direction. Since  $\boldsymbol{\Lambda}^1$  is comprised of piecewise polynomial differential 1-forms,  $\boldsymbol{\Lambda}^1$  and its derivatives are integrable in closed form along the straight path  $\mathbf{X}_\ell(t + \delta)$ . Thus, Eq. (5.68) defines a symplectic algorithm—specifically a gauge-compatible splitting method—that can be computed exactly.

### 5.3.6 Numerical Examples

The efficacy of this algorithm is now demonstrated numerically. First, a one-dimensional simulation of Landau damping electrons is considered, choosing simulation parameters similar to those of Xiao *et al.* [8], against a fixed, homogeneous, positive background charge. The 1X2V simulation approach pursued in Crouseilles

*et al.* [10] and Kraus *et al.* [15] is then reexpressed in canonical coordinates, thereby deriving the restriction of the foregoing algorithm to 1X2P phase space—comprised of one spatial dimension and two dimensions of canonical momentum. Finally the electromagnetic Weibel instability is simulated in this restricted phase space.

## Landau Damping

Using Whitney form finite elements, a 650-cell domain  $\mathcal{T}_h$  with periodic boundaries is constructed. Each cell is assigned width  $w_x = 2.4 \times 10^{-2}$  cm, and  $26 \times 10^6$  electrons are simulated (40,000 per cell, when unperturbed). With electron temperature at  $T_e = 5$  keV, the setup has Debye length  $\lambda_D = 1.0$  cm and plasma frequency  $\omega_p = 3.0 \times 10^9$  rad/s, roughly mirroring physical parameters of Xiao *et al.* [8].

The electric field is assumed to have initial perturbation at  $t = 0$

$$\mathbf{Y} = -\frac{\mathbf{E}}{4\pi c} = -\frac{E_0 \cos(kx)}{4\pi c} \hat{\mathbf{x}}, \quad (5.69)$$

where  $E_0 = 1.2$  statV/cm and  $k\lambda_D = 0.8$ . To construct this perturbation, the continuous 1-form field  $\mathbf{Y}_{\text{cont}}$  is first projected onto its Whitney form approximation, i.e.  $\mathbf{Y}_{\text{cont}} \xrightarrow{\pi_h} \mathbf{Y} = \mathbf{y} \cdot \mathbb{M}_1^{-1} \cdot \mathbf{\Lambda}^1$ . In particular,  $\mathbf{y}$  is solved for in Eq. (5.43) such that the integrals of  $\mathbf{Y}_{\text{cont}}$  and  $\mathbf{Y}$  agree on edges of the discretized domain. This procedure yields a sinusoidal  $\mu_{\text{field}} = \mathbb{G}^T \mathbf{y}$  as depicted in Fig. 5.1.

From the particle side, electron momenta are initialized in phase space by randomly selecting their velocities  $\dot{\mathbf{X}}_\ell$  from a Maxwellian distribution of temperature  $T_e = 5$  keV. Taking  $\mathbf{A} = 0$  at  $t = 0$ , initial canonical momenta are therefore given by  $\mathbf{P}_\ell = m_\ell \dot{\mathbf{X}}_\ell$ . Electron positions are then initialized to be consistent with Gauss' law. More precisely, the particle positions, in combination with the electric field perturbation, are generated to ensure the constancy of the total momentum map  $\mu$ . Following Eq. (5.63), a nonzero constant momentum map can be understood as a

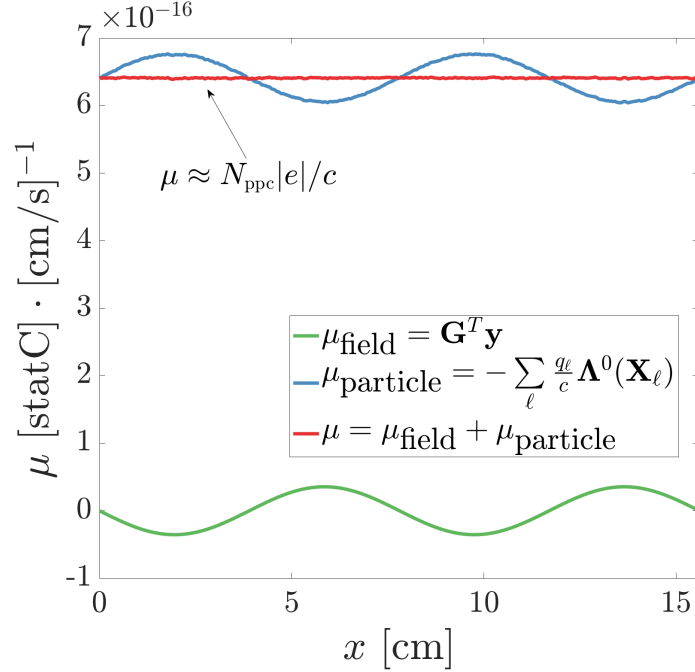


Figure 5.1: The terms of Eq. (5.61) are plotted over the simulation domain at time  $t = 0$ , characterizing initial conditions by the momentum map  $\mu = \mu_{\text{field}} + \mu_{\text{particle}}$ .

fixed, homogeneous, ion background charge,  $\mu \sim \rho_{\text{ext}}/c$ . Indeed, in a Landau damping simulation that takes only electrons to be dynamical, such a constant background charge constitutes the desired Gauss' law remainder.

The electron positions  $\{\mathbf{X}_\ell\}$  are therefore optimized to ensure that  $\mu_{\text{particle}} = \sum_\ell \frac{|e|}{c} \Lambda^0(\mathbf{X}_\ell)$  closely satisfies

$$\mu = \mu_{\text{field}} + \mu_{\text{particle}} \approx N_{\text{ppc}} |e| / c, \quad (5.70)$$

where  $\mu_{\text{field}} = \mathbb{G}^T \mathbf{y}$  and  $N_{\text{ppc}} = 40,000$  denotes the number of particles per cell. In this way, the positive background charge, characterized by  $\mu$ , is homogeneous across the simulation domain and enforces quasineutrality with the dynamical electrons.

This optimization of  $\mu_{\text{particle}}$  is carried out in two stages. First, electrons are

randomly selected via rejection sampling [107] from the distribution

$$n_e(x) = n_0 \left[ 1 + \frac{kE_0 \sin(kx)}{4\pi |e| n_0} \right], \quad (5.71)$$

which satisfies  $\nabla \cdot \mathbf{E} = 4\pi |e| (n_0 - n_e)$ . The electron positions  $\{\mathbf{X}_\ell\}$  are then further optimized using Nesterov accelerated gradient descent [108] to minimize the objective function

$$\arg \min_{\{\mathbf{X}_\ell\}} \left| \mu - \frac{N_{\text{ppc}} |e|}{c} \right|^2. \quad (5.72)$$

The resulting momentum map, plotted in red in Fig. 5.1, thus defines a background charge that is homogeneous to a high degree of accuracy.

Note that an alternative initialization, undertaken for example by Kraus *et al.* [15], reverses the above procedure by randomly generating electron positions first and then solving for  $\mathbf{y}$  to satisfy Gauss' law. This alternative is more straightforward computationally than the procedure described above, but it may afford less precision in the specification of the initial electric field perturbation, whenever such precision is desirable.

With initialized fields and electrons, the simulation is then evolved using a first order Lie-Trotter splitting [81] derived from Eq. (5.68), in particular,

$$\mathbf{u}(t + \Delta) = \exp(\Delta H_{\text{Kinetic}}^x) \exp(\Delta H_{\mathbf{Y}}) \exp(\Delta H_{\mathbf{A}}) \mathbf{u}(t) \quad (5.73)$$

where  $\mathbf{u}(t)$  denotes the simulation state at time  $t$ —i.e.  $\mathbf{u} = m_d \in M_d$ , a point in phase space as defined in Eq. (5.51).

In Fig. 5.2, the evolution of the momentum map is depicted throughout the simulation domain. Note that, while  $\mu_{\text{particle}}$  (multicolor) exhibits an oscillation and decay consistent with Landau damping,  $\mu$  (gray) remains constant over time, consistent

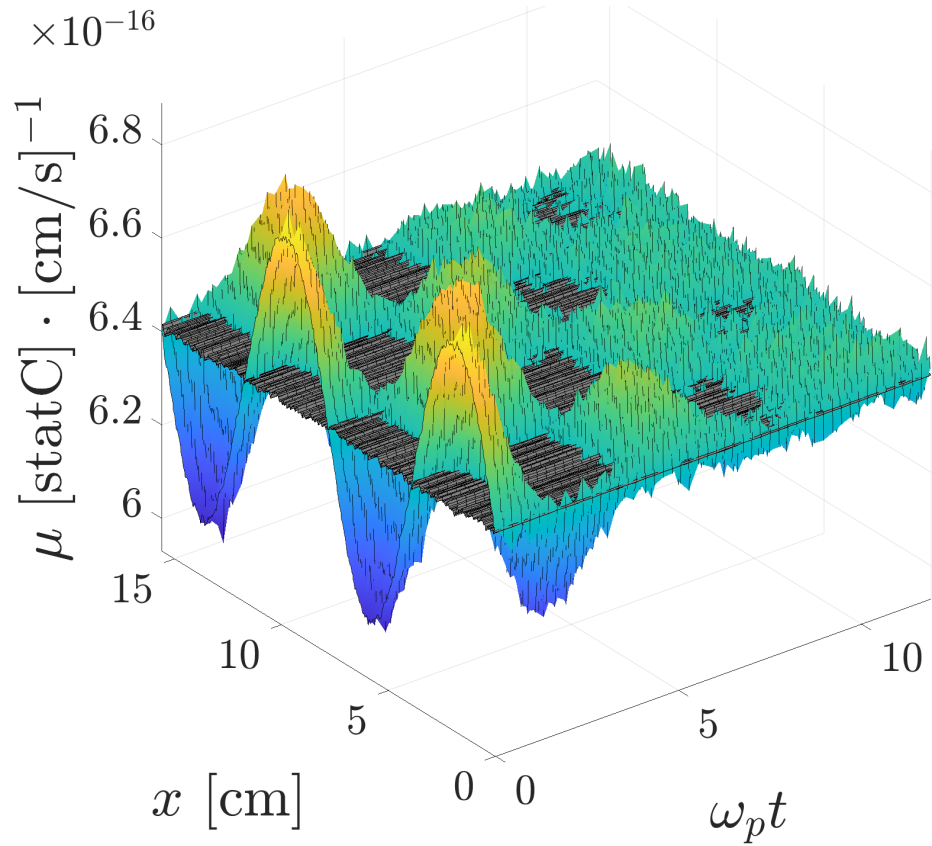


Figure 5.2: With their initial conditions as depicted in Fig. 5.1, the total momentum map  $\mu$  (gray) is compared with  $\mu_{\text{particle}}$  (multicolor) as the two functions evolve over time. Whereas  $\mu_{\text{particle}}$  exhibits a decaying sinusoid consistent with Landau damping,  $\mu$  remains constant to machine precision. The momentum map  $\mu$  constitutes a physical representation of the fixed positive background charge implicit in the simulation.

with the conservation of the momentum map.

To compare this simulation with theory, the evolution of the (normalized) electric field is plotted in Fig. 5.3, (which may be compared with Fig. 2 of Xiao *et al.* [8]). The results agree with a theoretical expectation of (i) electrostatic Langmuir wave oscillation at a frequency  $\omega_p = 3.0 \times 10^9$  rad/s, and (ii) Landau damping at a decay rate  $\omega_i = \frac{\omega_p}{\kappa^3} \sqrt{\frac{\pi}{8}} \exp\left(-\frac{1+3\kappa^2}{2\kappa^2}\right) = 3.9 \times 10^8$  rad/s, where  $\kappa = k\lambda_D$ . Furthermore, as is characteristic of a symplectic algorithm, the error in the total energy, measured by  $H_{\text{VM}}$  of Eq. (5.52), is well bounded throughout the simulation. This error is plotted in Fig. 5.4.

Having demonstrated the canonical finite element formalism’s efficacy in simulating an electrostatic problem, the electromagnetic simulation of the Weibel instability is next considered. Before that, however, the “canonical 1X2P phase space” is introduced, in which the simulation will be conducted.

### Canonical 1X2P Phase Space

Consider the restriction of phase space to one spatial dimension and two dimensions of canonical momentum. Despite its computational efficiency, the 1X2P setting is capable of simulating a number of nontrivial electromagnetic problems. The development here of 1X2P phase space essentially adapts for canonical coordinates the approach of Crouseilles *et al.* [10] and Kraus *et al.* [15].

To characterize 1X2P, the lack of  $y$  dependence must first be reflected in the finite element expansions of the fields. In this setting, therefore,  $\mathbf{A}$  and  $\mathbf{Y}$  are defined by analogy with Eq. (5.43) as

$$\begin{aligned}\mathbf{A} &= \mathbf{a}_x \cdot \boldsymbol{\Lambda}^1(x) + \mathbf{a}_y \cdot \boldsymbol{\Lambda}^0(x) \\ \mathbf{Y} &= \mathbf{y}_x \cdot \mathbb{M}_1^{-1} \cdot \boldsymbol{\Lambda}^1(x) + \mathbf{y}_y \cdot \mathbb{M}_0^{-1} \cdot \boldsymbol{\Lambda}^0(x).\end{aligned}\tag{5.74}$$

Here,  $\mathbf{a}_x$  denotes a vector of coefficients that pair only with the finite element 1-

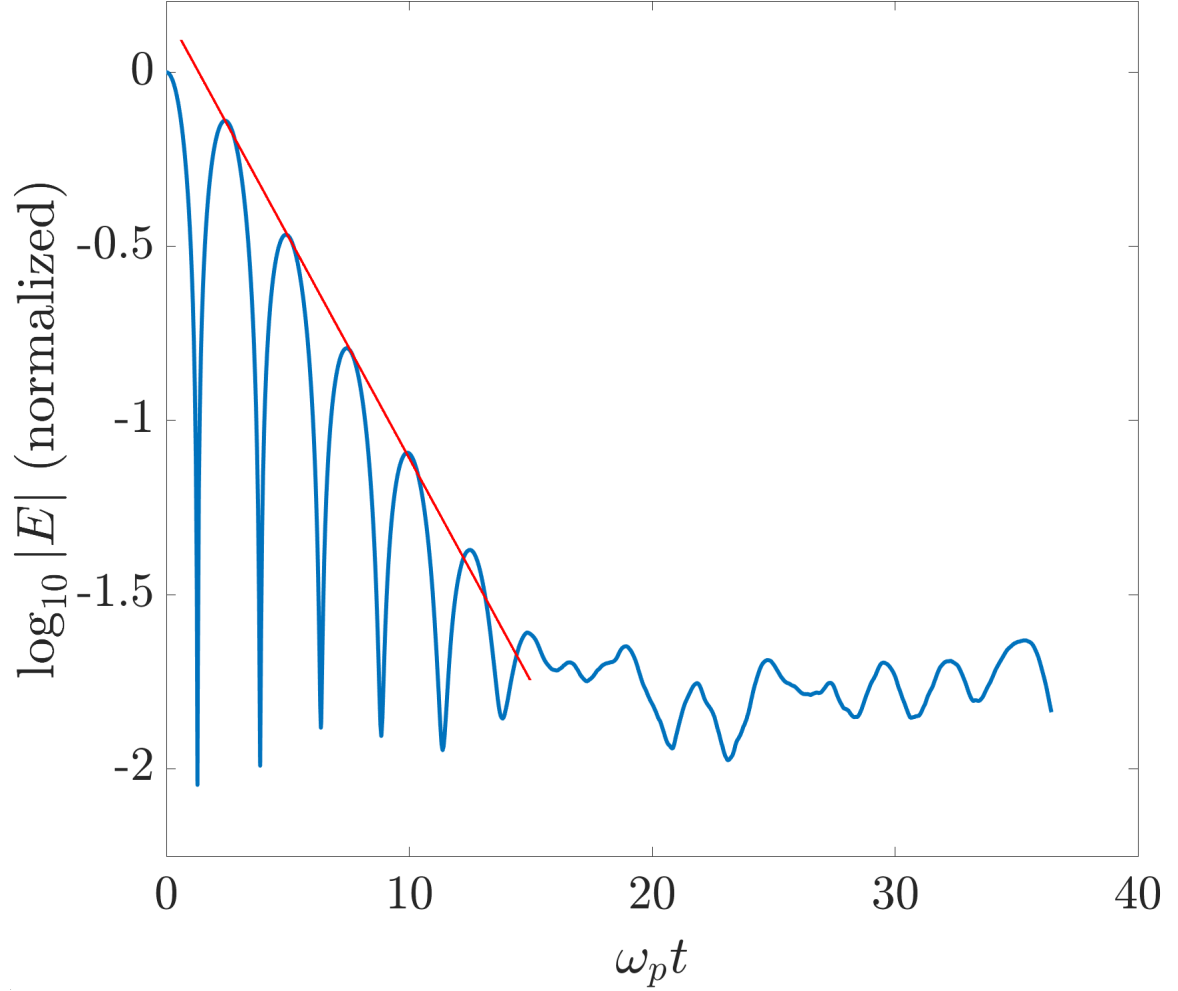


Figure 5.3: The evolution of an electrostatic wave over time is simulated with a first order Lie-Trotter splitting [81] of Eq. (5.68). The blue time series denotes the (normalized) log modulus of the electric field  $\mathbf{E} = -4\pi c\mathbf{Y}$ , where  $|\mathbf{E}|$  is computed over the simulation domain by the  $L^2\Lambda^1$  norm. The theoretical Landau damping rate of the wave in a Maxwellian plasma is depicted as a red line, decaying at a rate of  $\omega_i = \frac{\omega_p}{\kappa^3} \sqrt{\frac{\pi}{8}} \exp\left(-\frac{1+3\kappa^2}{2\kappa^2}\right)$  for  $\kappa = k\lambda_D$ .

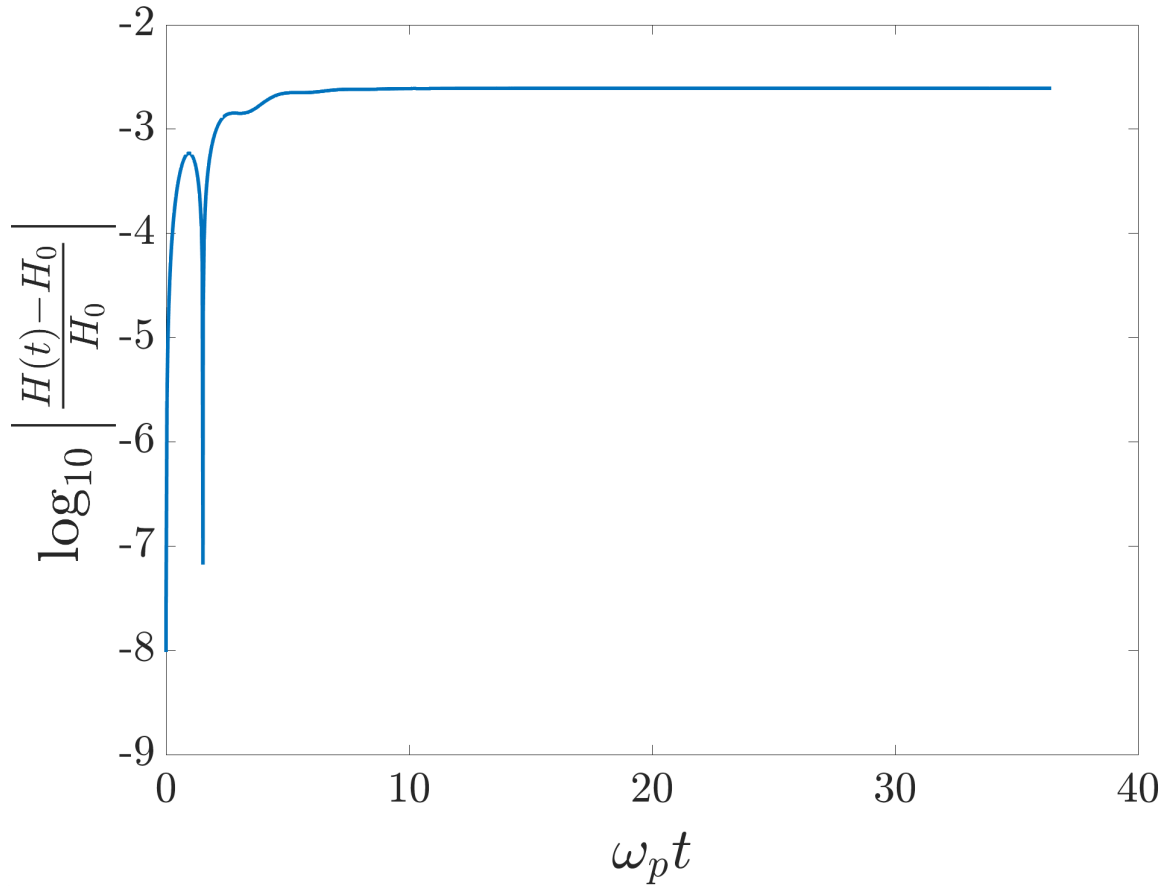


Figure 5.4: The log error in the total energy of a first order Lie-Trotter splitting [81] Landau damping simulation.

form basis  $\Lambda^1(x)$ —a basis in 1X2P which has only  $x$ -components and whose spatial dependence is only one-dimensional.  $\mathbf{a}_y$  is moreover defined as the coefficients of a  $0$ -form. Since there is no way to associate 1-forms with  $\hat{y}$ -directed edges in the 1X2P setting, 0-forms are the most natural representation of the  $y$  components of  $\mathbf{A}$ . This becomes especially clear when examining finite elements restricted to have spatial  $x$ -dependence. The expansion of  $\mathbf{Y}$  in Eq. (5.74) follows similarly, with appropriate mass matrices computed by integrals over the one-dimensional domain.

Turning now to the characterization of particle phase space, two components of the canonical momentum are retained,  $P_{\ell x}$  and  $P_{\ell y}$ . Only one component of spatial dependence is retained, which will be denoted  $X_\ell$ .

The appropriate Hamiltonian is then computed by restricting Eq. (5.52) as follows:

$$H_{1X2P} = \frac{1}{8\pi} \left( (4\pi c)^2 \left[ \mathbf{y}_x \cdot \mathbb{M}_1^{-1} \cdot \mathbf{y}_x + \mathbf{y}_y \cdot \mathbb{M}_0^{-1} \cdot \mathbf{y}_y \right] + \mathbf{a}_y \cdot \mathbb{G}^T \mathbb{M}_1 \mathbb{G} \cdot \mathbf{a}_y \right) + \sum_{\ell=1}^L \frac{1}{2m_\ell} \left( \left| P_{\ell x} - \frac{q_\ell}{c} \mathbf{a}_x \cdot \Lambda^1(X_\ell) \right|^2 + \left| P_{\ell y} - \frac{q_\ell}{c} \mathbf{a}_y \cdot \Lambda^0(X_\ell) \right|^2 \right). \quad (5.75)$$

Note that the term  $\mathbf{a}_x \cdot \mathbb{C}^T \mathbb{M}_2 \mathbb{C} \cdot \mathbf{a}_x$  is absent; while it would ordinarily arise from the magnetic energy  $|\mathbf{dA}|^2$ ,  $\mathbf{d}$  annihilates 1-forms in the 1X2P setting. Indeed, the magnetic field in the 1X2P formalism is given simply by  $\mathbf{B} = \mathbf{dA} = \mathbf{a}_y \cdot \mathbf{d}\Lambda^0 = \mathbb{C}\mathbf{a}_y \cdot \Lambda^1$ .

The Poisson bracket of the restricted phase space follows by simply omitting the inapplicable terms of Eq. (5.50). In particular:

$$\{F, G\}_{1X2P} = \left( \frac{\partial F}{\partial \mathbf{a}_x} \cdot \frac{\partial G}{\partial \mathbf{y}_x} + \frac{\partial F}{\partial \mathbf{a}_y} \cdot \frac{\partial G}{\partial \mathbf{y}_y} + \sum_{\ell=1}^L \frac{\partial F}{\partial X_\ell} \frac{\partial G}{\partial P_{\ell x}} \right) - (F \leftrightarrow G). \quad (5.76)$$

Observe that, despite its simplicity, the 1X2P phase space retains the gauge struc-

ture of the original problem. In particular, the gauge symmetry

$$\Phi_{\exp(\mathbf{s})} \begin{pmatrix} \mathbf{a}_x \\ P_{\ell x} \end{pmatrix} = \begin{pmatrix} \mathbf{a}_x + \mathbb{G}\mathbf{s}_x \\ P_{\ell x} + \frac{q_\ell}{c} \mathbb{G}\mathbf{s}_x \cdot \boldsymbol{\Lambda}^1(X_\ell)_x \end{pmatrix} \quad (5.77)$$

gives rise to the momentum map

$$\mu_{1X2P} = \mathbb{G}^T \mathbf{y}_x - \sum_{\ell=1}^L \frac{q_\ell}{c} \boldsymbol{\Lambda}^0(X_\ell). \quad (5.78)$$

Finally, the equations of motion may be derived in the 1X2P setting, which are straightforward reexpressions of their full phase space counterparts in Eq. (5.64):

$$\begin{aligned} \dot{X}_\ell &= \{X_\ell, H_{1X2P}\} = \frac{1}{m_\ell} \left( P_{\ell x} - \frac{q_\ell}{c} \mathbf{a}_x \cdot \boldsymbol{\Lambda}^1(X_\ell) \right) \\ \dot{P}_{\ell x} &= \{P_{\ell x}, H_{1X2P}\} = \frac{q_\ell}{c} \left[ \dot{X}_\ell \mathbf{a}_x \cdot (\partial_{X_\ell} \boldsymbol{\Lambda}^1(X_\ell)) + \dot{Y}_\ell \mathbf{a}_y \cdot (\partial_{X_\ell} \boldsymbol{\Lambda}^0(X_\ell)) \right] \\ \dot{\mathbf{a}}_x &= \{\mathbf{a}_x, H_{1X2P}\} = 4\pi c^2 \mathbb{M}_1^{-1} \cdot \mathbf{y}_x \\ \dot{\mathbf{a}}_y &= \{\mathbf{a}_y, H_{1X2P}\} = 4\pi c^2 \mathbb{M}_0^{-1} \cdot \mathbf{y}_y \\ \dot{\mathbf{y}}_x &= \{\mathbf{y}_x, H_{1X2P}\} = \sum_{\ell=1}^L \frac{q_\ell}{c} \dot{X}_\ell \boldsymbol{\Lambda}^1(X_\ell) \\ \dot{\mathbf{y}}_y &= \{\mathbf{y}_y, H_{1X2P}\} = \sum_{\ell=1}^L \frac{q_\ell}{c} \dot{Y}_\ell \boldsymbol{\Lambda}^0(X_\ell) - \frac{1}{4\pi} \mathbb{G}^T \mathbb{M}_1 \mathbb{G} \cdot \mathbf{a}_y. \end{aligned} \quad (5.79)$$

Here, with an abuse of notation that ignores the non-existence of  $Y_\ell$ ,  $\dot{Y}_\ell$  is used to denote

$$\dot{Y}_\ell = \frac{1}{m_\ell} (P_{\ell y} - \mathbf{a}_y \cdot \boldsymbol{\Lambda}^0(X_\ell)). \quad (5.80)$$

Observe that  $P_{\ell y}$  is conserved in Eq. (5.79), which can be viewed as a consequence of the independence from  $Y_\ell$  of the 1X2P formulation.

Further note that a gauge-compatible splitting of  $H_{1X2P}$  is readily defined by the

following four sub-Hamiltonians, in agreement with Eq. (5.66):

$$\begin{aligned}
H_{1X2P} &= H_{\mathbf{A}} + H_{\mathbf{Y}} + H_{\text{Kinetic}}^x + H_{\text{Kinetic}}^y \\
\text{where } H_{\mathbf{A}} &= \frac{1}{8\pi} \mathbf{a}_y \cdot \mathbb{G}^T \mathbb{M}_1 \mathbb{G} \cdot \mathbf{a}_y \\
H_{\mathbf{Y}} &= \frac{1}{8\pi} \left( (4\pi c)^2 \left[ \mathbf{y}_x \cdot \mathbb{M}_1^{-1} \cdot \mathbf{y}_x + \mathbf{y}_y \cdot \mathbb{M}_0^{-1} \cdot \mathbf{y}_y \right] \right) \\
H_{\text{Kinetic}}^x &= \sum_{\ell=1}^L \frac{1}{2m_\ell} \left| P_{\ell x} - \frac{q_\ell}{c} \mathbf{a}_x \cdot \boldsymbol{\Lambda}^1(X_\ell) \right|^2 \\
H_{\text{Kinetic}}^y &= \sum_{\ell=1}^L \frac{1}{2m_\ell} \left| P_{\ell y} - \frac{q_\ell}{c} \mathbf{a}_y \cdot \boldsymbol{\Lambda}^0(X_\ell) \right|^2.
\end{aligned} \tag{5.81}$$

Using the Poisson bracket  $\{\cdot, \cdot\}_{1X2P}$  of Eq. (5.76), the following subsystem equations of motion are thereby derived:

$$\begin{aligned}
H_{\mathbf{A}} : \left\{ \begin{array}{l} \dot{\mathbf{y}}_y = -\frac{1}{4\pi} \mathbb{G}^T \mathbb{M}_1 \mathbb{G} \cdot \mathbf{a}_y \end{array} \right. & \quad H_{\mathbf{Y}} : \left\{ \begin{array}{l} \dot{\mathbf{a}}_x = 4\pi c^2 \mathbb{M}_1^{-1} \cdot \mathbf{y}_x \\ \dot{\mathbf{a}}_y = 4\pi c^2 \mathbb{M}_0^{-1} \cdot \mathbf{y}_y \end{array} \right. \\
H_{\text{Kinetic}}^x : \left\{ \begin{array}{l} \dot{X}_\ell = \frac{1}{m_\ell} \left( P_{\ell x} - \frac{q_\ell}{c} \mathbf{a}_x \cdot \boldsymbol{\Lambda}^1(\mathbf{X}_\ell) \right) \\ \dot{P}_{\ell x} = \frac{q_\ell}{c} \dot{X}_\ell \mathbf{a}_x \cdot (\partial_{X_\ell} \boldsymbol{\Lambda}^1(X_\ell)) \\ \dot{\mathbf{y}}_x = \sum_{\ell=1}^L \frac{q_\ell}{c} \dot{X}_\ell \boldsymbol{\Lambda}^1(X_\ell) \end{array} \right. & \quad H_{\text{Kinetic}}^y : \left\{ \begin{array}{l} \dot{P}_{\ell x} = \frac{q_\ell}{c} \dot{Y}_\ell \mathbf{a}_y \cdot (\partial_{X_\ell} \boldsymbol{\Lambda}^0(X_\ell)) \\ \dot{\mathbf{y}}_y = \sum_{\ell=1}^L \frac{q_\ell}{c} \dot{Y}_\ell \boldsymbol{\Lambda}^0(X_\ell). \end{array} \right.
\end{aligned} \tag{5.82}$$

Since these equations of motion are—as Eq. (5.68)—exactly solvable, and since the sub-Hamiltonians of Eq. (5.81) preserve the gauge symmetry of Eq. (5.77), it is clear that Eq. (5.82) defines a gauge-compatible splitting method that exactly preserves  $\mu_{1X2P}$ .

## Weibel Instability

The 1X2P formulation defined above is now applied to the simulation of the Weibel instability. The simulation here is initialized in close agreement with the parametrization of the Weibel instability simulations of Crouseilles *et al.* [10] and Kraus *et al.* [15]. Specifically, in a periodic domain of 64 cells,  $N_e = 100,032$  electrons are simulated. Continuing to work in Gaussian units, the perturbation wavenumber is taken to be  $k = 1.25 \frac{\omega_p}{c}$  and a simulation domain length is given by  $L = 2\pi/k$ . A magnetic perturbation is instantiated by defining the initial vector potential to be

$$\mathbf{A} = \frac{B_0}{k} \sin(kx) \hat{y} \quad (5.83)$$

where  $B_0 = -5.7\text{mG}$ . Initial electron velocities are sampled from the anisotropic distribution

$$f_e(x, v_x, v_y) = \frac{1}{2\pi\sigma_x\sigma_y} \exp\left(-\left[\frac{v_x^2}{2\sigma_x^2} + \frac{v_y^2}{2\sigma_y^2}\right]\right) \quad (5.84)$$

where  $\sigma_x = 0.02c/\sqrt{2}$  and  $\sigma_y = \sqrt{12}\sigma_x$ . To initialize the initial electron distribution to be independent of  $x$  (i.e., spatially uniform) as above, electrons are evenly spaced throughout the simulation domain at separation of  $L/N_e$ .  $\mathbf{Y}$  is correspondingly initialized to zero.  $\mathbf{A}$  and  $\mathbf{Y}$  are again modeled using Whitney (0- and 1-) forms.

Finally, the Weibel instability is simulated with a Lie-Trotter splitting of stepsize  $1/40\omega_p$ , yielding the evolution plotted in Fig. 5.5. The magnetic field growth rate is in strong agreement with the analytic prediction [109],

$$\gamma = \frac{\omega_p k \sigma_y}{\sqrt{\omega_p^2 + c^2 k^2}}. \quad (5.85)$$

Lastly, the total energy is also well bounded over the lifetime of the Weibel instability simulation, as depicted in Fig. 5.6.

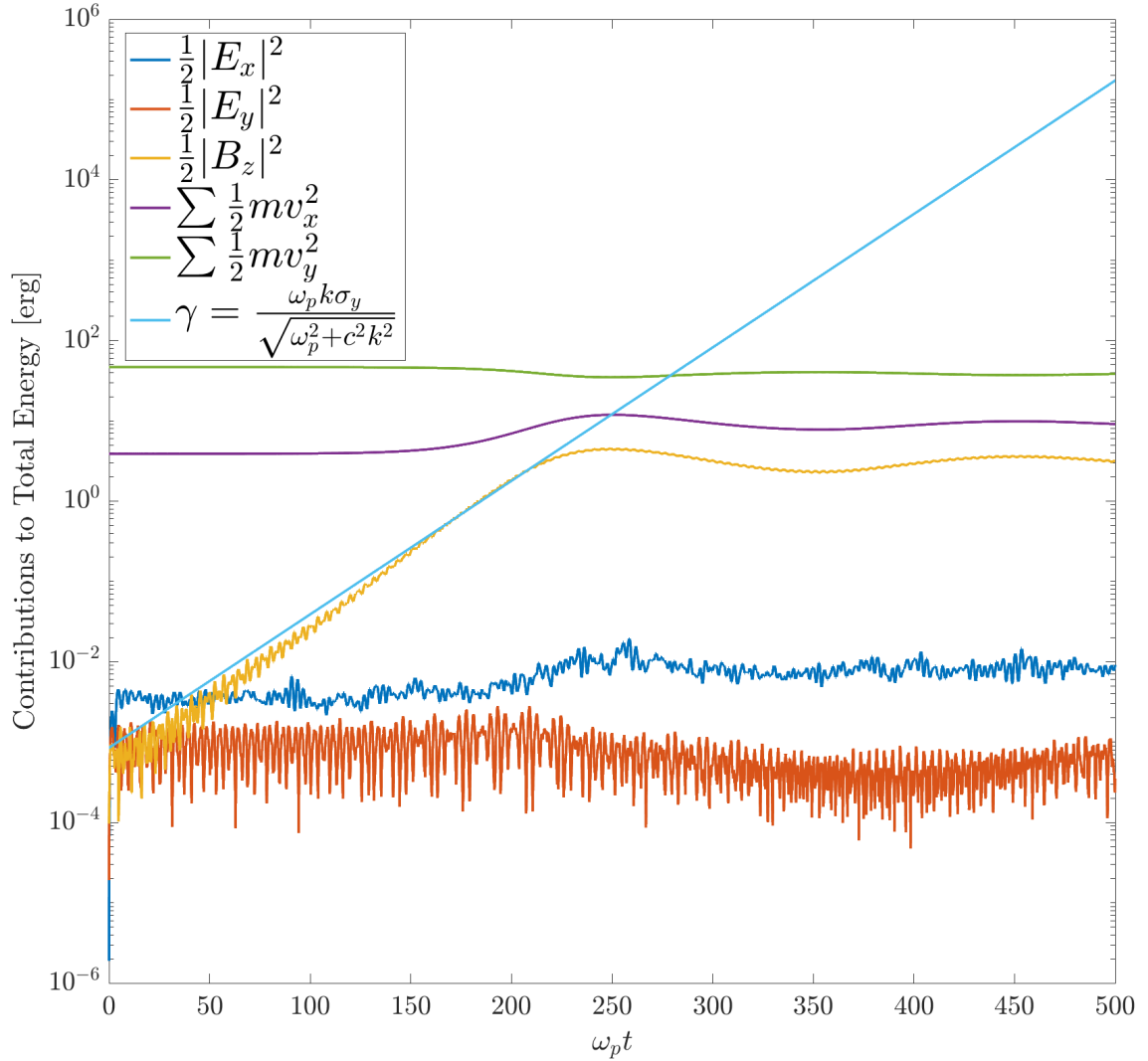


Figure 5.5: The growth rate of magnetic field energy closely approximates the analytic model of the Weibel instability. As the magnetic field ramps up, the anisotropy of electron velocity is reduced. This plot may be compared with Fig. 1 of Kraus *et al.* [15].

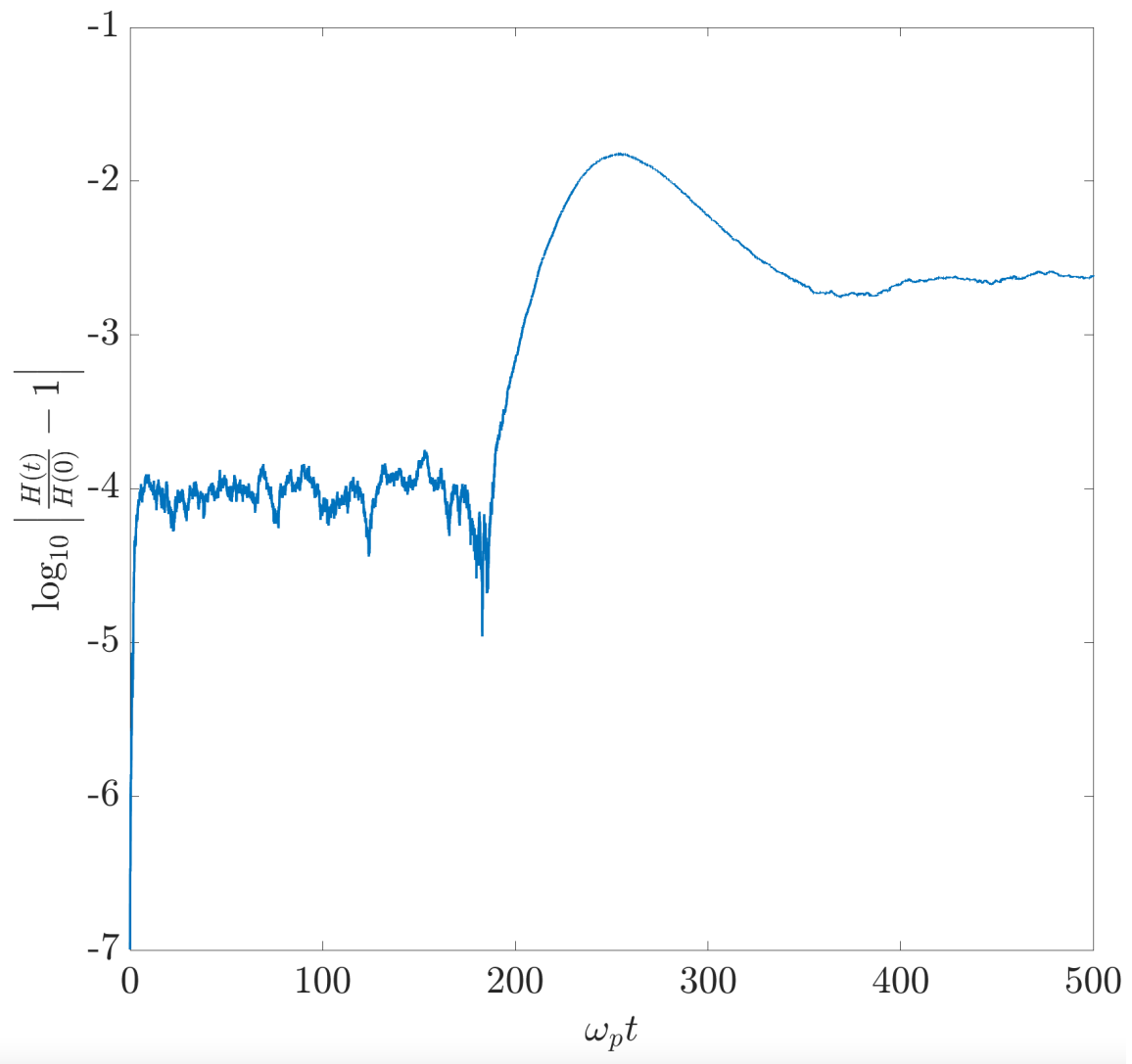


Figure 5.6: The log error in the total energy of a first order Lie-Trotter splitting [81] Weibel instability simulation [109].

## 5.4 N2T for a Vlasov-Maxwell variational algorithm via DEC

Shifting gears from the Hamiltonian to Lagrangian formalism, this section derives a charge conservation law for the discrete, gauge-symmetric variational Vlasov-Maxwell PIC method defined by Squire *et al.* [3]. In this PIC scheme, spacetime is discretized by a  $d$ -dimensional spatial simplicial complex (comprised of triangles in two dimensions or tetrahedra in three dimensions) whose structure is held constant throughout a uniformly discretized time. The time dimension may be envisaged as forming temporal edges that extend orthogonally from the spatial simplices, as in a triangular prism. This  $(d+1)$ -dimensional prismatic complex shall be denoted  $P_C$ . DEC [33] is employed to define fields on  $P_C$  that are single-valued on its  $k$ -cells (or their circumcentric duals) for  $0 \leq k \leq d + 1$ . Here, a spatial dimensionality of  $d = 3$  shall be assumed, so that  $P_C$  is four-dimensional, with three-dimensional spatial tetrahedra comprising each time slice.

Following the construction of cochains briefly reviewed in Section 4.1, the electromagnetic gauge field  $A$ —a discrete 1-form defined on all edges of  $P_C$ —neatly splits in into an electric potential  $\phi_{n-\frac{1}{2}}^i := -A_{n-\frac{1}{2}}^i$  and a vector potential  $\mathbf{A}_n^{ij} := A_n^{ij}$ , as follows:

$$\begin{aligned}
 A &= - \sum_{i,n} \phi_{n-\frac{1}{2}}^i \Delta_{n-\frac{1}{2}}^i + \sum_{[ij],n} \mathbf{A}_n^{ij} \Delta_n^{ij} \\
 &= -\phi_{e_t} \Delta^{e_t} + \mathbf{A}_{e_s} \Delta^{e_s}.
 \end{aligned}
 \tag{5.86}$$

Using Eq. (4.4),  $dA$  may correspondingly be expressed as:

$$\begin{aligned}
dA &= -\phi_{e_t} d\Delta^{e_t} + \mathbf{A}_{e_s} d\Delta^{e_s} \\
&= (-\phi_{e_t} W_{f_t}^{e_t} + \mathbf{A}_{e_s} W_{f_t}^{e_s}) \Delta^{f_t} + \mathbf{A}_{e_s} W_{f_s}^{e_s} \Delta^{f_s} \\
&= E \wedge dt + B \\
&= F,
\end{aligned} \tag{5.87}$$

where  $dt$  denotes the 1-form  $dt := \sum_{e_t} \Delta^{e_t}$  and where the wedge product is used to implicitly define the spatial 1- and 2-forms  $E$  and  $B$  and the Faraday 2-form  $F$  [110]. (As a note of caution, in keeping with DEC conventions, the preceding vector potential  $\mathbf{A}$  is a single number on each spatial edge. Its bold notation is only suggestive. On the other hand, the Whitney interpolant of  $\mathbf{A}$  will be seen to coordinatize  $\mathbb{R}^3$  and thereby extend the single-valued  $\mathbf{A}$  from the spatial edges of  $P_C$  to a 3-component vector field.)

Now, the discrete action of Squire *et al.* [3] is defined on  $P_C$  by

$$\begin{aligned}
S &= \sum_{V_{\sigma^2}} -\frac{1}{2} dA \wedge \star dA + \sum_{p,n} \left\{ \frac{h}{2} m_p \left| \frac{\mathbf{X}_{n+\frac{1}{2}}^p - \mathbf{X}_{n-\frac{1}{2}}^p}{h} \right|^2 - q_p \sum_i \phi_{n-\frac{1}{2}}^i \varphi^i(\mathbf{X}_{n-\frac{1}{2}}^p) \right. \\
&\quad \left. + q_p \left( \frac{\mathbf{X}_{n+\frac{1}{2}}^p - \mathbf{X}_{n-\frac{1}{2}}^p}{h} \right) \cdot \sum_{[ij]} \mathbf{A}_n^{ij} \int_{t_{n-\frac{1}{2}}}^{t_{n+\frac{1}{2}}} dt \varphi^{ij}(\mathbf{X}^p(t)) \right\}.
\end{aligned} \tag{5.88}$$

In Eq. (5.88), a sum over support volumes has been denoted  $V_{\sigma^2}$  for the primal-dual 4-form  $dA \wedge \star dA$ , with  $A$  defined as in Eq. (5.86).  $V_{\sigma^2}$  represents the convex hull of the 2-chain  $\sigma^2$  and its dual  $\star\sigma^2$  on which  $\langle dA, \sigma^2 \rangle$  and  $\langle \star dA, \star\sigma^2 \rangle$  are respectively defined. The symbol  $h$  denotes the time step,  $n$  the time index and  $p$  the particle index.  $\mathbf{X}^p(t)$  is defined as the constant velocity path between the particle's staggered-time positions  $\mathbf{X}_{n-\frac{1}{2}}^p$  and  $\mathbf{X}_{n+\frac{1}{2}}^p$ . In particular, particle paths are chosen to have straight

line trajectories between the staggered times  $t \in [(n - \frac{1}{2})h, (n + \frac{1}{2})h]$ ,  $\forall n \in \mathbb{Z}$ .

The Whitney 0-form  $\varphi^i(x)$  and 1-form  $\varphi^{ij}(x)$  interpolate  $\phi$  and  $\mathbf{A}$  to an arbitrary point  $x \in P_C$  [36, 37]. In effect,  $\varphi^i$  and  $\varphi^{ij}$  complete the spatial components of the cochain bases  $\Delta_n^i$  and  $\Delta_n^{ij}$  adopted in Eq. (4.2) by extending DEC forms to the convex hull of  $P_C$ . In the continuous spacetime of the Klimontovich-Maxwell system, the everywhere-defined gauge fields  $\phi(t, \mathbf{x})$  and  $\mathbf{A}(t, \mathbf{x})$  were ‘attached’ to point particles by the delta function,  $\delta^{(3)}(\mathbf{x} - \mathbf{X}_j(t))$ . In the prismatic complex  $P_C$ , Whitney forms play this role by interpolating the gauge fields to the locations of point particles. Likewise, while geometric notions are not ascribed to any point particles themselves, Whitney forms on  $P_C$  attach geometry to the charge densities and currents of the particles, as did the delta function in Eq. (3.101). For example, the spatial dot product in Eq. (5.88) composes  $\mathbf{X}_{n+\frac{1}{2}}^p$  with the Whitney-interpolated 3-component vector field  $\mathbf{A}_n^{ij} \varphi^{ij}(\mathbf{X}^p(t))$ , (where  $\mathbf{A}_n^{ij}$  represents a single number and  $\varphi^{ij}$  a 3-component vector).

Now following the continuous spacetime N2T procedure of Eqs. (3.99)-(3.106), the equations of motion and gauge symmetry of  $S$  in Eq. (5.88) are examined. As previously seen, the differential structure of spacetime has been replaced in the discrete setting by the prismatic complex  $P_C$ , its DEC operators and Whitney forms. To derive the Euler-Lagrange equations of  $S$ , therefore, Euler operators must be defined for fields on the discrete DEC structure. By analogy with Eq. (3.81), such an operator must implement a variational derivative on the space of fields defined on  $P_C$ .

Consider, for example, a  $k$ -form  $\alpha$  defined by its expansion in  $k$ -cochain basis elements:  $\alpha = \sum_{\sigma} \alpha_{\sigma} \Delta^{\sigma}$ , where  $\sigma$  ranges over all  $k$ -cells on  $P_C$ . Since each component  $\alpha_{\sigma}$  of  $\alpha$  can be varied independently and only algebraically in the action  $S$ , the variational derivative of  $\alpha_{\sigma}$  takes the simple form of a partial derivative. The Euler

operator  $\mathbf{E}_{\alpha_\sigma}$  on the action  $S$  can therefore be straightforwardly defined as follows:

$$\begin{aligned}\mathbf{E}_{\alpha_\sigma}(S) &:= \frac{\partial S}{\partial \alpha_\sigma} \\ &= \frac{\partial}{\partial \alpha_\sigma} \sum L.\end{aligned}\tag{5.89}$$

Note that in a discrete setting, variational derivatives are best construed to act on the entire action  $S$ , rather than on the Lagrangian, because discrete Lagrangians are necessarily non-local. As usual it will be assumed that all fields and their variations have compact support, such that any divergence term in  $L$ —which contributes to  $S = \sum L$  only at the boundary—vanishes under  $\mathbf{E}_{\alpha_\sigma}$ . Eq. (5.89) is the DEC counterpart to the continuous Euler operator defined in Eq. (3.81), and is now applied to derive equations of motion.

To calculate  $\mathbf{E}_{\phi_{e_t}}(S)$  and  $\mathbf{E}_{\mathbf{A}_{e_s}}(S)$ ,  $dA \wedge \star dA$  is first reexpressed in  $S$  using Eqs. (2.81)-(2.86) and the invariance of  $S$  under the addition of a divergence ( $L \rightarrow L + d\gamma$ )

$$dA \wedge \star dA \stackrel{(2.81)}{=} (dA, dA) \mathbf{vol}_\eta \stackrel{(2.86)}{\approx} (A, \delta dA) \mathbf{vol}_\eta \stackrel{(2.81)}{=} A \wedge \star \delta dA \stackrel{(2.84)}{=} A \wedge d \star dA,\tag{5.90}$$

where  $\approx$  indicates equality up to an (ignorable) divergence. Then, using Eq. (5.86) and noting the symmetry of the intermediate expression  $(dA, dA) \mathbf{vol}_\eta$  above, the Euler operator of Eq. (5.89) is applied to derive the equations of motion for  $A$  as follows:

$$0 = \mathbf{E}_{\phi_{e_t}}(S) = \Delta^{e_t} \wedge d \star dA - \rho^{e_t}\tag{5.91a}$$

$$0 = \mathbf{E}_{\mathbf{A}_{e_s}}(S) = -\Delta^{e_s} \wedge d \star dA + J^{e_s}\tag{5.91b}$$

where

$$\rho^{e_t} := \sum_p q_p \varphi^i \left( \mathbf{X}_{t(e_t)}^p \right) \quad (5.92a)$$

$$J^{e_s} := \sum_p q_p \left( \frac{\mathbf{X}_{t_f(e_s)}^p - \mathbf{X}_{t_i(e_s)}^p}{h} \right) \cdot \int_{t_i(e_s)}^{t_f(e_s)} dt \varphi^{e_s} (\mathbf{X}^p(t)). \quad (5.92b)$$

In Eq. (5.92a),  $i$  denotes the spatial vertex associated with  $e_t$ , and  $\mathbf{X}_{t(e_t)}^p$  denotes the position of particle  $p$  at the time coincident with the midpoint  $\left[ n - \frac{i}{2} \right]$  of  $e_t$ . In Eq. (5.92b),  $\mathbf{X}_{t_i(e_s)}^p$  and  $\mathbf{X}_{t_f(e_s)}^p$  denote the initial and final particle positions, respectively, coincident with the midpoints  $\left[ n - \frac{i}{2} \right]$  and  $\left[ n + \frac{i}{2} \right]$  that bookend the  $t = n$  time slice containing  $e_s$ .

It is worth pausing to interpret these equations of motion. First observe that the primal-dual wedge product in Eq. (5.91a) is only non-vanishing on the spatial ( $\star \Delta^{e_t}$ ) component of  $d \star dA$ . This follows from the definition of the primal-dual wedge product, which is only non-zero on the convex hulls of a cell and its dual:  $CH(\sigma, \star \sigma)$ . Reading off from Eq. (5.87), therefore, Eq. (5.91a) becomes

$$\rho^{e_t} = \Delta^{e_t} \wedge d \star (E \wedge dt) = dD \wedge \Delta^{e_t}, \quad (5.93)$$

Gauss's law for the electric displacement dual 2-form  $D$ , as expected. An analogous interpretation of Eq. (5.91b) yields a discrete Ampère-Maxwell law. The  $\mathbf{E}_{\mathbf{X}^p}(S)$  equations of motion for particle trajectories have been omitted, as they will not be necessary for the derivation of charge conservation via N2T—just as they were unnecessary in Eqs. (3.105)-(3.106). These implicit time-step particle equations of motion are derived in [3].

Having derived the field equations of motion, the gauge symmetry of the action  $S$  in Eq. (5.88) must now be examined. In particular,  $S$  is invariant under the local

gauge transformation  $A \rightarrow A - df$ , defined by

$$\begin{aligned}\phi_{n+\frac{1}{2}}^i &\rightarrow \phi_{n+\frac{1}{2}}^i + \delta\phi_{n+\frac{1}{2}}^i = \phi_{n+\frac{1}{2}}^i + (f_{n+1}^i - f_n^i) \\ \mathbf{A}_n^{ij} &\rightarrow \mathbf{A}_n^{ij} + \delta\mathbf{A}_n^{ij} = \mathbf{A}_n^{ij} - (f_n^j - f_n^i),\end{aligned}\tag{5.94}$$

where  $f = f_v \Delta^v$  is an arbitrary primal 0-form on  $P_C$ .

After all, the electromagnetic term of  $S$ — $dA \wedge \star dA$ —is clearly invariant under  $A \rightarrow A - df$ , since  $d^2 = 0$ . Furthermore, as noted in Squire *et al.* [3], the gauge invariance of the particle terms of  $S$  follows from the defining property of Whitney interpolation noted in Eq. (4.7), namely:  $d_c((\alpha)_{\text{interp}}) = (d_d \alpha)_{\text{interp}}$ , where  $d_c$  and  $d_d$  denote continuous and discrete exterior derivatives, respectively and  $(\cdot)_{\text{interp}}$  denotes Whitney interpolation. Eq. (5.94) therefore transforms  $L \rightarrow L + d_c \gamma$ , adding a divergence term analogous to the transformation of Eq. (3.104) for the continuous spacetime Vlasov-Maxwell system.

Following Eq. (3.103), the gauge transformation of Eq. (5.94) is seen to be generated by a vector field

$$\mathbf{v}_f = \sum_{\alpha} Q^{\alpha}[f] \partial_{u^{\alpha}} = \sum_{e_t} (d_{e_t} f) \partial_{\phi_{e_t}} - \sum_{e_s} (d_{e_s} f) \partial_{\mathbf{A}_{e_s}},\tag{5.95}$$

where the coefficient  $d_e f = f_{v_2} - f_{v_1}$  corresponds to the oriented edge  $e = [v_1 v_2]$ , and where the sums are taken over all temporal and spatial edges, respectively.

Thus, the data sufficient to complete the N2T construction of Eq. (3.89) has been gathered for the DEC system. As in Eq. (3.105), the characteristics of the symmetry

and equations of motion combine to form

$$\begin{aligned}
\sum_{\alpha} Q^{\alpha}[f] \mathbf{E}_{u^{\alpha}}(S) &= \sum_{e_t} Q^{\phi_{e_t}}[f] \cdot \mathbf{E}_{\phi_{e_t}}(S) + \sum_{e_s} Q^{\mathbf{A}_{e_s}}[f] \cdot \mathbf{E}_{\mathbf{A}_{e_s}}(S) \\
&= \sum_{e_t} (d_{e_t} f) \cdot \left( \Delta^{e_t} \wedge d \star dA - \rho^{e_t} \right) \\
&\quad + \sum_{e_s} (-d_{e_s} f) \cdot \left( -\Delta^{e_s} \wedge d \star dA + J^{e_s} \right).
\end{aligned} \tag{5.96}$$

Now note that

$$(d_e f) \Delta^e = d(f_v \Delta^v) = df, \tag{5.97}$$

so applying the Euler operator for  $f_v$  at vertex  $v = \begin{bmatrix} i \\ n \end{bmatrix}$  to Eq. (5.96) yields

$$\begin{aligned}
0 &= \mathbf{E}_{f_v} \left[ \sum_{\alpha} Q^{\alpha}[f] \mathbf{E}_{u^{\alpha}}(S) \right] \\
&= \mathbf{E}_{f_v} \left[ \sum_{V_{\sigma^1}} df \wedge d \star dA - \sum_{e_t} (d_{e_t} f) \cdot \rho^{e_t} - \sum_{e_s} (d_{e_s} f) \cdot J^{e_s} \right] \\
&= \Delta^v \wedge \star d \star dA + \left( \rho_{n+\frac{1}{2}}^i - \rho_{n-\frac{1}{2}}^i \right) + \sum_j J^{[ij]} \\
&= \left( \rho_{n+\frac{1}{2}}^i - \rho_{n-\frac{1}{2}}^i \right) + \sum_j J^{[ij]}
\end{aligned} \tag{5.98}$$

since up to a sign,  $(\delta \star d) = (\star d \star d) = \star d^2 = 0$ . The sum of  $J^{[ij]}$  over  $j$  captures all spatial edges that terminate on vertex  $v = \begin{bmatrix} i \\ n \end{bmatrix}$ .

The last equality of Eq. (5.98) reveals the desired charge conservation law on  $P_C$ . By its very construction through N2T, this conservation law is guaranteed to be an off-shell differential identity, as was Eq. (3.106). This fact may be verified as follows.

First, restrict sources  $\rho$  and  $J$  to a particle of charge  $q$  whose path over one time step remains within a single spatial tetrahedron; the general case follows without significant alteration. Then, note [36, 37] that the Whitney 0-form  $\varphi^i$  interpolates

from vertex  $i$  via barycentric coordinates such that, over the tetrahedron  $[ijkl]$ ,

$$\varphi^i + \varphi^j + \varphi^k + \varphi^\ell = 1. \quad (5.99)$$

In vector form, the 1-form  $\varphi^{ij}$  is then given by

$$\varphi^{ij} = \varphi^i \nabla \varphi^j - \varphi^j \nabla \varphi^i. \quad (5.100)$$

Summing over the three spatial edges terminating on vertex  $i$  of the tetrahedron containing the particle, therefore

$$\begin{aligned} \sum_{j \neq i} \varphi^{ij} &= \varphi^i \nabla \left( \sum_{j \neq i} \varphi^j \right) - \left( \sum_{j \neq i} \varphi^j \right) \nabla \varphi^i \\ &= \varphi^i \nabla (1 - \varphi^i) - (1 - \varphi^i) \nabla \varphi^i \\ &= -\nabla \varphi^i. \end{aligned} \quad (5.101)$$

It follows, then, that

$$\begin{aligned} \sum_{j \neq i} J^{[ij]} &= q \left( \frac{\mathbf{X}_f - \mathbf{X}_i}{h} \right) \cdot \int_{t_i}^{t_f} dt \sum_{j \neq i} \varphi^{ij}(\mathbf{X}(t)) \\ &= -q \left( \frac{\mathbf{X}_f - \mathbf{X}_i}{h} \right) \cdot \int_{t_i}^{t_f} dt \nabla \varphi^i(\mathbf{X}(t)) \\ &= -q \int_i^f \mathbf{v} \lrcorner d\varphi^i \\ &= -q [\varphi^i(\mathbf{X}_f) - \varphi^i(\mathbf{X}_i)] \end{aligned} \quad (5.102)$$

where  $\mathbf{v} \lrcorner d\varphi^i$  is the interior product of the exact form  $d\varphi^i$  with respect to the velocity  $\mathbf{v} := \frac{1}{h}(\mathbf{X}_f - \mathbf{X}_i)$ , which is constant over a single time step of the particle. Upon comparison with the definition for  $\rho$  in Eq. (5.92a), it is clear that Eq. (5.98) holds off-shell, as desired. The N2T formalism of [40] has succeeded in deriving the

off-shell, discrete conservation law.

As a final note, an alternative approach to deriving the conservation law of the DEC Vlasov-Maxwell action—Eq. (5.88)—entails gauge fixing this action by setting  $\phi_{n+\frac{1}{2}}^i = 0$ . Such a gauge fixing would remove the system’s degeneracy and uniquely determine solutions to its equations of motion (which otherwise require a gauge choice when the algorithm is evolved). In such an approach, N1T would be applied to the time-*independent* symmetry transformation  $\mathbf{A}(t, \mathbf{x}) \rightarrow \mathbf{A}(t, \mathbf{x}) - \nabla\psi(\mathbf{x})$  (or its DEC equivalent  $\mathbf{A}_n^{ij} \rightarrow \mathbf{A}_n^{ij} - (f_n^j - f_n^i)$  as in Eq. (5.94). Thus, a non-trivial conservation law in the form of a time evolution of Gauss’s law would be found. The Hamiltonian counterpart to this procedure was studied in the previous two sections, which both worked in a fixed temporal gauge and derived the corresponding momentum map.

# 6

## Conclusion

### 6.1 Thesis summary

This dissertation is rooted in the study of structure-preserving algorithms for plasma physics, a discipline that lies at the intersection of computational and mathematical physics. Structure-preserving algorithms preserve salient mathematical features of the underlying physical systems they model. This work, in particular, focuses on the algorithmic preservation of gauge-structure, that is, the symmetries and conservation laws that serve as crucial descriptors of a physical system. Leveraging insights from this study, this dissertation discovers new particle-in-cell algorithms for plasma physics and characterizes their effective preservation of gauge symmetry and electric charge.

Examining gauge structure in a setting that is not original—especially, in algorithmic approximations of physical laws rather than in the setting of the laws themselves—emphasizes the significant ‘supporting structure’ required to preserve gauge structure. In particular, an algorithm’s preservation of variational or symplectic structure, and its respect for the topological properties of the underlying system, both appear prerequisite for the preservation of gauge structure.

In essence, this dissertation is about Noether’s theorems, and demonstrating their applicability beyond variational systems in continuous spacetime. It defines a new, general class of Hamiltonian algorithms that rigorously uphold the Noether principle, and it also demonstrates how Noether’s theorems can be successfully applied in new variational discretization schemes. Moreover, this dissertation helps clarify why some of the algorithms that have already appeared in the literature have been so successful. Lastly, this work contributes new algorithms to the literature, and demonstrates their efficacy via numerical simulation.

As a final note, the results of this thesis convey an overall impression of the adaptability of gauge theories to the discrete structures of algorithms. Internal gauge symmetries are characterized by the transformation of fields defined against the background of spacetime, and their geometric structure can therefore be maintained even after the algorithmic discretization of this background. The present effort demonstrates that much of the formalism that gauge theories employ—whether in Lagrangian or Hamiltonian systems—is readily ported to discrete settings more suitable for computation.

## 6.2 Main results

More specifically, this work discovers gauge-compatible splitting methods, a general class of Hamiltonian algorithms that requires each sub-Hamiltonian of a splitting method to be exactly solvable and gauge-symmetric. Such algorithms exactly preserve the momentum map of a physical system, and are generalizable to any Hamiltonian system with gauge symmetry. The momentum map further serves as an important guide for the precise setting of initial conditions; in the case of a gauge-invariant PIC method, the momentum map’s systematic definition of charge density enables the precise assignment (or, avoidance) of ‘external’ fixed charges in a simulation.

Gauge compatible splitting methods further reveal the decided advantage of splitting methods over alternative time discretizations of Hamiltonian systems.

Secondly, this general class is applied to the construction of two particle-in-cell Hamiltonian splitting algorithms, both of which are defined with a canonical Poisson structure. The first is set on a cubic mesh using interpolation functions that are required—by the demands of gauge structure—to satisfy the properties of Whitney forms. Its Gauss’ law momentum map is found, and the method is demonstrated to be gauge-compatible, so that the momentum map exactly preserved. Using this momentum map, the symplectic reduction of this algorithm is further studied, revealing the relationship between this algorithm and those in the existing literature.

The second algorithm is constructed using finite element exterior calculus, rendering it suitable for simulation on an unstructured mesh. It is tested numerically against an example of Landau damping, demonstrating the machine-precision preservation of its momentum map, and the strong agreement between theoretical expectations and simulation outcome. It is demonstrated that the momentum map can be regarded as an external fixed charge in a PIC simulation. Using this interpretation, the initial conditions of a Landau damping simulation were optimized to precisely model a homogeneous positive fixed background charge. This algorithm is further tested in a demonstration of the Weibel instability, demonstrating the effect of electron temperature anisotropy in a genuinely electromagnetic (as opposed to electrostatic) problem. The expected analytic growth rate of the magnetic field is recovered to high accuracy.

Lastly, Noether’s second theorem is demonstrated for a variational PIC method in the formalism of discrete exterior calculus. The method discovers an off-shell charge continuity equation for the primal complex setting of the algorithm, which, due to its discrete setting, conveys meaningful information about the flow of charge through the simulation.

### 6.3 Future work

There are several potential extensions of this work that are possible. First, the gauge-compatible splitting PIC methods defined in this dissertation are structure-preserving and explicitly solvable and, as a result, can be efficiently scaled and assured of their performance in long-time simulations. Consequently, such algorithms are well-poised to capitalize on the high-performance scientific computing architecture now available.

Second, the identification of the momentum map in such algorithms enables their precise initialization of PIC simulations requiring fixed background charges. Such a technique might be advantageous, for example, in the simulation of plasma interactions with charged plasma-facing components.

Third, the flexibility of finite element exterior calculus makes it significantly generalizable as well. For example, the FEEC PIC algorithm developed here, which is suitable for simulations on an unstructured mesh, may be adapted to simulations using curvilinear coordinates.

Fourth, the successful adaptation of structure-preserving algorithms for particle-in-cell methods could be pushed to alternative representations of kinetic plasmas. For example, the direct discretization of the Vlasov-Maxwell system does not represent kinetic plasmas via point particles, but rather by an evolving distribution in phase space. It would be interesting to extend the lessons of this thesis to a characterization of such a system's Poisson structure (or almost Poisson structure).

Fifth, this dissertation has focused primarily on the electromagnetic gauge symmetry of plasmas. But this is only one of eleven smooth symmetries enjoyed by a classical plasma. The other ten are the spacetime symmetries of the Poincaré group. Preserving these symmetries in algorithms for plasma physics might enable a simulation of plasmas that exactly conserves energy-momentum.

This final topic is undertaken in the appendices of this thesis, where some prelim-

inary results are achieved.

# Appendix A

## Overview of Appendices

This dissertation is born of a desire to understand and demonstrate the ability of plasma simulation algorithms to preserve the symmetry of their underlying models. The results of the preceding chapters make a case for the naturalness of gauge structure in discrete algorithms for plasma physics. But of the eleven smooth symmetries that essentially characterize physical models of plasmas, only one of them—electromagnetic gauge symmetry—is an internal gauge symmetry.

These four appendices grapple with the remaining ten—the spacetime symmetries. The strategy pursued in each appendix is to leverage the remarkable compatibility of gauge symmetry with discrete algorithms. To this end, the spacetime symmetries, which are ordinarily viewed as symmetries of the spacetime manifold, are reinterpreted as internal, vertical symmetries at a fixed point.

Before proceeding with the appendices, a brief summary of their strategies, successes, and pitfalls is provided here.

### **Appendix B** [49]

- Strategy: In the manner of lattice gauge theory, construct an identity-valued loop, a  $\mathbb{1}$ -loop, on a hypercubic lattice to replace a Yang-Mills-type equation— $\delta\Omega + j = 0$ —with a Lie group-valued counterpart— $\delta\Omega \cdot J = \mathbb{1}$ . Use a Wilson

loop for  $\Omega$ , and find suitable lattice definitions for the 5-vector matter current  $J$ , and the covariant codifferential,  $\delta$ .

- Successes: A natural current  $J$  is found that appropriately transforms in the adjoint representation. A  $\mathbb{1}$ -loop is defined that recovers a known Poincaré gauge theory of gravity in its continuum limit.
- Pitfalls: No suitable definition of  $\delta$  is found that ensures Poincaré invariance.

### Appendix C

- Strategy: Extend  $\mathbb{1}$ -loop theory to a representation that can incorporate Poincaré symmetry and  $U(1)$  symmetry.
- Successes: A  $U(2,2)$  representation is found, inspired by the twistor theory of Roger Penrose. It is noted that, as defined, the current  $J$  is at most a rank 2 matrix, and therefore has a “spectrum” with only certain permissible combinations of Lie algebra elements.
- Pitfalls: Since  $SU(2,2)$  is the conformal group, alongside the eleven Poincaré and  $U(1)$  symmetries appear five more: a dilation and four special conformal transformations.

### Appendix D [50]

- Strategy: Construct a Lorentz invariant discretization of the tetradic Palatini action using the Poincaré representation of 5-vector theory.
- Successes: A tetradic Palatini action in vacuum is indeed identified, and its equations of motions are derived.
- Pitfalls: It is unclear how this method can be extended to the simulation of matter evolving under gravity.

# Appendix B

## 1-Loop Theory

### B.1 Introduction

In this appendix, a formalism is developed [49] that attempts to reconcile Poincaré invariance with a discrete, but otherwise classical, universe. Our own motivation for this work arises from a desire to formulate algorithms that exactly conserve energy and momentum in simulations of classical physical systems. Because the spacetimes of algorithms are necessarily discrete, and the Noether symmetries [38] they model necessarily continuous, vital conservation laws are generally broken in any first principles simulation. This forfeiture of spacetime symmetry is a central challenge of computational physics, whose resolution bears upon questions of theoretical physics as well.

1-loop (‘one-loop’) theory is here introduced as a formalism for a lattice gauge theory of the Poincaré group,  $\mathbb{P} = \mathbb{T}^{3,1} \rtimes SO^+(3, 1)$ . We adopt an unconventional view of Poincaré symmetry that identifies  $\mathbb{P}$  as a gauge group of foreground physical fields, rather than the symmetry group of a background spacetime. We correspondingly regard the lattice of 1-loop theory as a mere graph, rather than an embedding in a continuous spacetime possessing dimensionality and extent.

The dynamical framework we adopt relinquishes Lagrangian and Hamiltonian formalism, and instead reformulates Yang-Mills [111] equations of motion directly in a discrete, gauge-invariant construct we call the  $\mathbb{1}$ -loop. The  $\mathbb{1}$ -loop generalizes the Wilson loop [112] and derives its physics from a conserved current  $\mathcal{J}$ , rather than a Lagrangian  $\mathcal{L}$  or Hamiltonian  $\mathcal{H}$ .  $\mathbb{1}$ -loop dynamics are described not by pointwise-defined differential equations— $E(\mathcal{L}) = 0$  or  $\frac{d}{dt} = \{\cdot, \mathcal{H}\}$ , say—but by finite lattice loops of Lie group elements whose composition evaluates to the identity:  $[g_1 \cdots g_n](\mathcal{J}) = \mathbb{1}$ .

Briefly, the basic  $\mathbb{1}$ -loop for a gauge group  $G$  is

$$\delta\Omega \cdot J = \mathbb{1}. \tag{B.1}$$

This relation recovers its Yang-Mills counterpart in the continuous spacetime limit,

$$\delta DA + j = 0. \tag{B.2}$$

The current  $J$  and holonomy  $\Omega$  of Eq. (B.1) are  $G$ -valued lattice loops, and  $\mathbb{1} \in G$  denotes the identity.  $\delta$  in Eq. (B.1) is a covariant codifferential redefined as a map between  $G$ -valued loops, satisfying  $\delta^2\Omega = \mathbb{1}$  and  $(\delta\alpha)^{-1} = \delta(\alpha^{-1}) \forall \alpha$ . Thus,  $\delta J = \mathbb{1}$  follows from Eq. (B.1). This  $\mathbb{1}$ -loop conservation law forms a lattice counterpart to the Yang-Mills relation  $\delta j = 0$ . Whereas Yang-Mills theories are defined for compact, reductive gauge groups, however,  $\mathbb{1}$ -loop theory is designed for the gauge groups of reductive Cartan geometries [43, 113], such as  $\mathbb{P}$ .

To construct a  $\mathbb{1}$ -loop theory of the Poincaré group, a  $\mathbb{P}$ -valued current  $J$  must be defined. In fact, by requiring that currents transform in the adjoint representation of  $\mathbb{P}$ , the  $\mathbb{1}$ -loop formalism uniquely determines  $J$  from a mere choice of matter field. In this work,  $J$  is thereby constructed from a recently defined Poincaré representation, the 5-vector  $\Phi$  [47, 48]. The  $\mathbb{P}$ -valued holonomy  $\Omega$  is likewise formed from a Poincaré gauge field,  $A$ . Finally, leveraging ideas from Cartan geometry, we shall define the

operator  $\delta$  in a manner comparable to the Wilson loop reconstruction of the covariant derivative  $D$ .

The resulting 1-loop theory constitutes a lattice Poincaré gauge theory of gravity. We will demonstrate that in the torsionless continuum limit, this theory recovers Einstein’s vacuum equations and its fields evolve along geodesics. In the appropriate limit, therefore, Poincaré 1-loop theory accords with general relativity [114] in vacuum. In the presence of matter, however, torsion and angular momentum play important dynamical roles in 1-loop theory—as they do in most Poincaré gauge theories of gravity [115–127]. We shall contextualize 1-loop theory within this existing literature. In its continuum limit, 1-loop theory will be seen to recover the field equations of a less-studied Poincaré gauge theory [122–127].

## B.2 A Motivating Aside: Dynamical Variables for Gauge Theories

We briefly review an argument [128] for the naturalness of Wilson loops as dynamical variables for gauge fields. The experimentally-confirmed Aharonov-Bohm effect [129] demonstrates that the 2-form Faraday tensor  $F(x) \in \Lambda^2[M, \mathfrak{u}(1)]$  under-describes the effects of the electromagnetic gauge field. On the other hand, the gauge field  $A(x) \in \Lambda^1[M, \mathfrak{u}(1)]$  over-describes them:  $A(x)$  can be freely gauge-transformed without physical consequence. Physical gauge-theoretic dynamical variables are therefore to be found somewhere ‘between’  $A$  and  $F$ .

For abelian gauge theories, the group-valued Wilson loop [41]

$$W_C = P \exp \left[ i \oint_C A(x) \right] \tag{B.3}$$

satisfies both criteria of a dynamical variable; it is gauge-invariant and captures the

Aharonov-Bohm effect. In non-abelian gauge theories, however,  $W_C$  generally transforms nontrivially under a gauge transformation; although the path-ordering operator  $P$  ensures the gauge invariance of  $W_C$  at all intermediate points of the loop  $C$ , its basepoint  $x_0$  leads  $W_C$  to transform as the adjoint  $g(x_0)W_Cg^{-1}(x_0)$ . As a result, the invariant dynamical variable in non-abelian gauge theories is defined by the trace of Eq. (B.3), that is,  $\text{Tr}[W_C]$ .

In the present effort, we pursue a slightly different strategy in defining physical variables. In particular, we define group-valued loops that evaluate to the identity element  $\mathbb{1}$ , as follows:

$$\mathbb{1}_C = P \exp \left[ i \oint_C (A|j)(x) \right] = \mathbb{1}. \quad (\text{B.4})$$

In this expression, we have generalized the integrand of Eq. (B.3), allowing it to be either the gauge field  $A(x)$  or the current  $j(x)$ , depending on the point  $x \in C$ . Like the gauge field, the current  $j(x)$  of an arbitrary gauge theory is a  $\mathfrak{g}$ -valued 1-form [42]. As such,  $\mathbb{1}_C$  generalizes the Wilson loop to allow for its dependence on  $j(x) \in \Lambda^1[M, \mathfrak{g}]$ , while restricting it to be identity-valued. In what follows, we refer to a loop in the form of Eq. (B.4) as a  $\mathbb{1}$ -loop. When  $\mathbb{1}$ -loops are defined on a lattice, they serve as discrete, gauge-invariant counterparts to classical physics' pointwise-defined differential equations of motion.

Unlike  $W_C$ , the  $\mathbb{1}$ -loop is invariant in an arbitrary gauge theory; because of its identity value,  $\mathbb{1}_C$  is gauge-invariant for abelian and non-abelian groups alike.  $\mathbb{1}_C$  may also be inverted or cyclically permuted without penalty; neither the orientation nor the basepoint  $x_0$  of  $C$  affects its evaluation to  $\mathbb{1}$ .

We emphasize two additional properties of  $\mathbb{1}_C$ , shared by  $W_C$ . First, whereas  $F(x)$  is evaluated at a point in spacetime, the spatio-temporal extent of the loop  $C$  is non-vanishing. This motivates Wilson's exploration of gauge theories on a discrete

lattice, where loops are necessarily non-vanishing and perhaps more readily defined. Second,  $\mathbb{1}_C$  and  $W_C$  both reveal the naturalness of working with Lie group elements rather than Lie algebra elements. For example, an observed phase difference in the Aharonov-Bohm experiment only fixes the integral in Eq. (B.3) up to integer multiples of  $2\pi$ . Its Lie algebra value is therefore unobservable and indeterminate, while its corresponding group element, by contrast, is fully specified.

### B.3 Attempting a 1-loop $U(1)$ Lattice Gauge Theory

We first attempt to construct a 1-loop theory from a familiar gauge theory—scalar QED. We begin by recalling its classical equations of motion, derived from the Lagrangian  $\mathcal{L} = -(\mathbb{D}^\mu\phi)^*(\mathbb{D}_\mu\phi) - m^2\phi^*\phi - \frac{1}{4}F^{\mu\nu}F_{\mu\nu}$  in continuous  $\mathbb{R}^{3,1}$  spacetime with flat metric  $g_{\mu\nu}(x) = \eta_{\mu\nu}$  of signature  $(-+++)$ :

$$\mathbb{D}^\mu F_{\mu\nu} + ej_\nu = 0 \tag{B.5a}$$

$$(\mathbb{D}^\mu\mathbb{D}_\mu - m^2)\phi = 0, \tag{B.5b}$$

where  $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ ,  $\mathbb{D}_\mu\phi = (\partial_\mu - ieA_\mu)\phi$ , and  $A_\mu dx^\mu \in \Lambda^1[\mathbb{R}^{3,1}, \mathfrak{u}(1)]$ . Like the gauge field, the current  $j_\mu = i[(\mathbb{D}_\mu\phi)^*\phi - \phi^*(\mathbb{D}_\mu\phi)]$  is a  $\mathfrak{u}(1)$ -valued 1-form,  $j_\mu dx^\mu \in \Lambda^1[\mathbb{R}^{3,1}, \mathfrak{u}(1)]$ . For convenience, we recall that  $\mathbb{D}^\mu F_{\mu\nu} = \partial^\mu F_{\mu\nu}$  due to the trivial abelian adjoint action of  $g \in U(1)$  on  $X \in \mathfrak{u}(1)$ , that is,  $\text{Ad}_g X = gXg^{-1} = X$ .

Our strategy requires that all dynamical equations are re-expressed as 1-loops in the form of Eq. (B.4). To that end, we first restate the gauge field equation of motion

by formally exponentiating the  $\mathbf{u}(1)$ -valued Eq. (B.5a):

$$\exp(D^\mu F_{\mu\nu} + e j_\nu) = \mathbb{1}. \quad (\text{B.6})$$

While identity-valued, as desired, this relation for the pointwise-defined Faraday tensor  $F_{\mu\nu}$  must be further re-expressed as a loop integral of  $A_\mu$  and  $j_\mu$ , as in Eq. (B.4).

We therefore reconstruct Eq. (B.6) on a hypercubic lattice  $\{\mathbf{n}\} = \mathbb{Z}^4$ , letting Greek indices  $\{\alpha, \beta, \dots\}$  correspond to lattice directions  $\{t, x, y, z\}$ . First, we derive a discrete form of Eq. (B.5a) from a lattice action  $S$  defined over  $\mathbb{Z}^4$ :

$$S = \sum_{\mathbf{n} \in \mathbb{Z}^4} \left[ -\frac{1}{4} F^{\mu\nu}[\mathbf{n}] F_{\mu\nu}[\mathbf{n}] + e j_\mu[\mathbf{n}] A^\mu[\mathbf{n}] \right], \quad (\text{B.7})$$

where  $F_{\mu\nu} = d_\mu^+ A_\nu[\mathbf{n}] - d_\nu^+ A_\mu[\mathbf{n}]$  with finite difference operator  $d_\mu^\pm f[\mathbf{n}] = \pm(f[\mathbf{n} \pm \hat{\mu}] - f[\mathbf{n}])$ . For now, we regard  $j_\mu[\mathbf{n}]$  as arbitrary and independent of  $A^\nu$ . Setting  $\partial S / \partial A^\nu[\mathbf{n}] = 0$ , we derive the following discrete gauge field equation of motion from Eq. (B.7):

$$\eta^{\mu\sigma} d_\mu^- F_{\sigma\nu}[\mathbf{n}] + e j_\nu[\mathbf{n}] = 0. \quad (\text{B.8})$$

We now substitute the left-hand side of Eq. (B.8) into the exponent of Eq. (B.6) to discover the following  $\mathbb{1}$ -loop on  $\mathbb{Z}^4$ :

$$\begin{aligned} \mathbb{1}_\nu[\mathbf{n}] &= J_\nu[\mathbf{n}] \prod_{\mu \neq \nu} G_\nu^\mu[\mathbf{n}] \\ &= J_\nu[\mathbf{n}] \prod_{\mu \neq \nu} \left( U^\mu{}_\nu[\mathbf{n}] U^{-\mu}{}_\nu[\mathbf{n}] \right) = \mathbb{1}. \end{aligned} \quad (\text{B.9})$$

This expression may be compared with Eq. (B.4). It is a  $\mathbb{1}$ -loop reformulation of Maxwell's equations in the desired form,  $[g_1 \cdots g_n](j) = \mathbb{1}$ . In Eq. (B.9),  $\nu$  is fixed

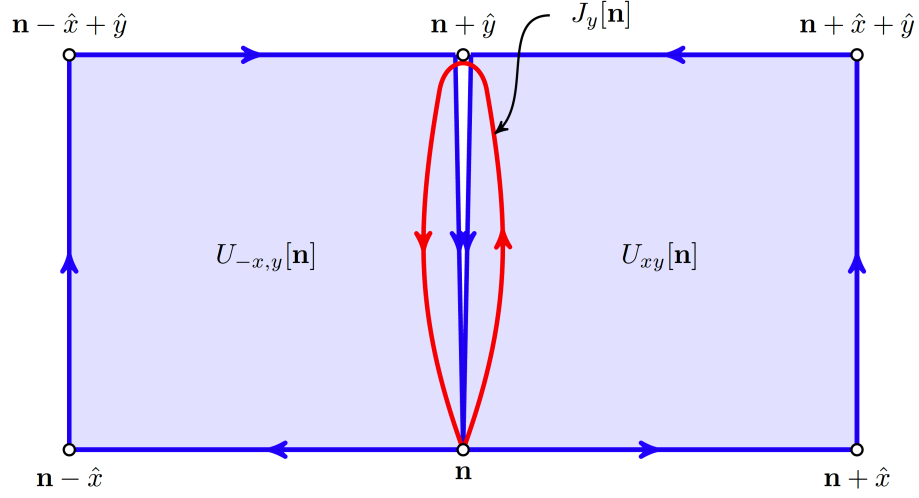


Figure B.1: Noting the positive spatial signature of the metric  $\eta_{\mu\nu}$ , we depict  $G_y^x[\mathbf{n}] = U_{xy}[\mathbf{n}]U_{-x,y}[\mathbf{n}]$  and  $J_y[\mathbf{n}]$ . The current  $J_y[\mathbf{n}]$  forms a round-trip loop along lattice edge  $[\mathbf{n}|\mathbf{n} + \hat{y}]$ . A  $\mathbb{1}$ -loop is thus formed by  $J_y[\mathbf{n}]G_y^t[\mathbf{n}]G_y^x[\mathbf{n}]G_y^z[\mathbf{n}] = \mathbb{1}$ .

and we have defined

$$\begin{aligned}
 G_\nu^\mu[\mathbf{n}] &= U_\nu^\mu[\mathbf{n}]U_\nu^{-\mu}[\mathbf{n}] \\
 U_{\pm\mu}^{\pm\mu}[\mathbf{n}] &= \exp(\eta^{\mu\mu} \log U_{\pm\mu,\nu}[\mathbf{n}]) \\
 U_{\mu\nu}[\mathbf{n}] &= U_\nu[\mathbf{n}]^{-1}U_\mu[\mathbf{n} + \hat{\nu}]^{-1}U_\nu[\mathbf{n} + \hat{\mu}]U_\mu[\mathbf{n}] \\
 U_\mu[\mathbf{n}] &= \exp(iA_\mu[\mathbf{n}]) \\
 J_\mu[\mathbf{n}] &= \exp(iej_\mu[\mathbf{n}]).
 \end{aligned} \tag{B.10}$$

We have used the fact that  $U(1)$  is abelian to freely factor the exponentiation of Eq. (B.8). For  $\mu = t$ , we note that  $U_\nu^\mu[\mathbf{n}] = U_{\mu\nu}[\mathbf{n}]^{-1}$ . A depiction of  $J_y[\mathbf{n}]$  and  $G_y^x[\mathbf{n}]$  is rendered in Fig. B.1.

Two obstructions to a  $U(1)$   $\mathbb{1}$ -loop theory are now seen plain. The first is, in part, aesthetic: The metric structure of Maxwell's equations is rather shoehorned into Eq. (B.10). Beyond our desire to recover Eq. (B.8), there is no geometric motivation for the appearance of  $\eta^{\mu\mu}$  in  $U_{\pm\mu}^{\pm\mu}[\mathbf{n}]$ , nor is there a readily apparent generalization

of Eq. (B.9) for a curved metric  $g_{\mu\nu}$ .

Second, although the 1-loop of Eq. (B.9) defines the desired dynamics for the  $U(1)$  gauge field of lattice scalar QED, a complete field theory must also specify dynamics for the matter field  $\phi[\mathbf{n}]$  (and  $j_\mu[\mathbf{n}]$  therewith). For example, a variational Lagrangian approach might derive intuitive lattice discretizations of Eq. (B.5b), such as [130]

$$[\mathbb{1} - S^{-\mu} e^{ieA_\mu[\mathbf{n}]}]_\mu [e^{-ieA_\mu[\mathbf{n}]} S^\mu - \mathbb{1}]^\mu \phi[\mathbf{n}] - m^2 \phi[\mathbf{n}] = 0, \quad (\text{B.11})$$

where  $S^{\pm\mu} (e^{A_\nu[\mathbf{n}]} f[\mathbf{n}]) = e^{A_\nu[\mathbf{n} \pm \hat{\mu}]} f[\mathbf{n} \pm \hat{\mu}]$  defines the shift operator  $S^{\pm\mu}$ , and a Minkowski-signed sum over  $\mu$  is implicit.

However, while Eq. (B.9) formulates the gauge field equation of motion as a 1-loop, Eq. (B.11) is not of this form. Indeed, because the matter field equation of motion—Eq. (B.5b)—is not Lie-algebra-valued, it offers no such re-expression. To define a 1-loop theory, therefore, whose dynamical equations can only be expressed as 1-loops, we must find an alternative group-valued representation of matter field dynamics.

A solution to this impasse is suggested by the following observation: The vanishing divergence of the energy-momentum tensor nearly enforces a system's equations of motion. This may be seen for Klein-Gordon and Dirac field theories as follows:

$$\begin{aligned} \partial^\mu T_{\mu\nu}^\phi &= \partial^\mu [\partial_\mu \phi \partial_\nu \phi + \eta_{\mu\nu} \mathcal{L}^\phi] \\ &= \partial_\nu \phi [\partial^2 \phi - m^2 \phi] \\ \partial^\mu T_{\mu\nu}^\psi &= \partial^\mu [i\bar{\psi} \gamma_\mu \partial_\nu \psi - \eta_{\mu\nu} \mathcal{L}^\psi] \\ &= \partial_\nu \bar{\psi} [-i\gamma^\mu \partial_\mu \psi + m\psi] + [i\partial_\mu \bar{\psi} \gamma^\mu + m\bar{\psi}] \partial_\nu \psi, \end{aligned} \quad (\text{B.12})$$

where we have defined  $2\mathcal{L}^\phi = -\partial^\sigma \phi \partial_\sigma \phi - m^2 \phi^2$  and  $\mathcal{L}^\psi = i\bar{\psi} \gamma^\sigma \partial_\sigma \psi - m\bar{\psi} \psi$ . We conclude from Eq. (B.12) that, wherever the matter fields  $\phi$  and  $\psi$  are non-constant, their respective equations of motion are enforced by energy-momentum conservation—

that is, by  $\mathbb{T}^{3,1}$  translation symmetry. (A similar result obtains in theories of fluids when their dynamical equations are written in conservative form.) In this sense, the energy-momentum tensor contains comparable information to a theory's Lagrangian or Hamiltonian.

Thus, for a gauge theory of a group  $G \supset \mathbb{T}^{3,1}$ , matter field dynamics may be determined by its  $G$ -valued conservation law. To address both aforementioned obstructions, therefore, we shall apply the preceding construction of  $U(1)$  theory toward a  $\mathbb{1}$ -loop lattice gauge theory of the Poincaré group,  $\mathbb{P} = \mathbb{T}^{3,1} \rtimes SO^+(3, 1)$ . We will form a ten-component, Poincaré-valued energy-momentum  $\mathcal{J}$  from a Poincaré representation—the 5-vector  $\Phi$ . In lieu of applying variational derivatives to derive Euler-Lagrange equations  $E[\mathcal{L}(\Phi)] = 0$ , or a Poisson bracket to derive flows  $\dot{\Phi} = \{\Phi, \mathcal{H}\}$ , we shall construct a  $\mathbb{1}$ -loop to discover the dynamics of  $\Phi$  from  $\mathcal{J}$ . We thereby recover matter field dynamics from a  $\mathbb{P}$ -valued  $\mathbb{1}$ -loop lattice gauge theory, whose gravitational dynamics will be explored in the continuum limit.

## B.4 $\mathbb{1}$ -loop Poincaré Gauge Theory

We first define the Poincaré representation  $\Phi$  on the hypercubic infinite lattice  $\{\mathbf{n}\} = \mathbb{Z}^4$ . We let Latin indices  $a, b, \dots \in \{t, x, y, z\}$  correspond to lattice directions and let Greek indices  $\alpha, \beta, \dots \in \{0, 1, 2, 3\}$  denote internal Lorentz degrees of freedom. Following [47, 48], we define the 5-vector  $\Phi[\mathbf{n}]$  to be a 5-component vector at lattice

vertex  $\mathbf{n} \in \mathbb{Z}^4$  that gauge transforms under local Poincaré transformations, as follows:

$$\begin{aligned}
\Phi'[\mathbf{n}] &= g[\mathbf{n}] \triangleright \Phi[\mathbf{n}] \\
&= (\Lambda, \varphi)[\mathbf{n}] \triangleright \Phi[\mathbf{n}] \\
&= \begin{bmatrix} \Lambda^\mu{}_\nu & \mathbf{0} \\ \varphi_\nu & 1 \end{bmatrix} \begin{bmatrix} \pi^\nu \\ \phi \end{bmatrix} \\
&= \begin{bmatrix} \Lambda^\mu{}_\nu \pi^\nu \\ \phi + \varphi_\nu \pi^\nu \end{bmatrix}.
\end{aligned} \tag{B.13}$$

Here,  $'$  denotes a gauge transformation,  $\triangleright$  denotes a left group action, and  $[\mathbf{n}]$  is often omitted for brevity. Thus,  $\Phi[\mathbf{n}]$  is a real representation of the Poincaré group,  $\mathbb{P} \rightarrow GL_5(\{\Phi\}, \mathbb{R})$ , a transpose of the Bargmann representation [51] of spacetime transformations. The 5-vector formalism was previously adopted in the Duffin-Kemmer system [131], however, the gauge transformation of Eq. (B.13) has not been identified in such work.

We next describe a Poincaré gauge field along the lattice links of  $\mathbb{Z}^4$ . We let  $\mathfrak{p} = \text{Lie}(\mathbb{P})$ ,  $\mathfrak{h} = \text{Lie}(H)$  and  $\mathfrak{t} = \text{Lie}(\mathbb{T}^{3,1})$  denote Lie algebras, where  $H = SO^+(3, 1)$ . We define the lowered-index vierbein  $e_{\mu a}[\mathbf{n}] = \eta_{\mu\nu} e^\nu{}_a[\mathbf{n}]$  to be a  $\mathfrak{t}$ -valued translation gauge field on the link  $[\mathbf{n}|\mathbf{n} + \hat{a}]$ . We likewise define the  $\mathfrak{h}$ -valued gauge field  $\Gamma^\mu{}_{\nu a}[\mathbf{n}]$ , which couples to  $e_{\mu a}[\mathbf{n}]$  through the group action of  $\mathbb{P}$ . To establish notation, we

thereby construct a covariant derivative of the 5-vector as follows:

$$\begin{aligned}
D_a^+ \Phi[\mathbf{n}] &= \Phi_a^+[\mathbf{n}] - \Phi[\mathbf{n}] \\
&= U_a[\mathbf{n}]^{-1} \cdot \Phi[\mathbf{n} + \hat{a}] - \Phi[\mathbf{n}] \\
\begin{bmatrix} D_a^+ \pi^\mu[\mathbf{n}] \\ D_a^+ \phi[\mathbf{n}] \end{bmatrix} &= \begin{bmatrix} (\pi_a^+)^{\mu}[\mathbf{n}] \\ \phi_a^+[\mathbf{n}] \end{bmatrix} - \begin{bmatrix} \pi^\mu[\mathbf{n}] \\ \phi[\mathbf{n}] \end{bmatrix} \\
&= \exp \begin{bmatrix} \Gamma_{\nu a}^{\mu}[\mathbf{n}] & \mathbf{0} \\ e_{\nu a}[\mathbf{n}] & 0 \end{bmatrix}^{-1} \begin{bmatrix} \pi^\nu \\ \phi \end{bmatrix} [\mathbf{n} + \hat{a}] - \begin{bmatrix} \pi^\mu \\ \phi \end{bmatrix} [\mathbf{n}].
\end{aligned} \tag{B.14}$$

A backward covariant derivative is analogously defined:

$$\begin{aligned}
D_a^- \Phi[\mathbf{n}] &= \Phi[\mathbf{n}] - \Phi_a^-[\mathbf{n}] \\
&= \Phi[\mathbf{n}] - U_a[\mathbf{n} - \hat{a}] \cdot \Phi[\mathbf{n} - \hat{a}].
\end{aligned} \tag{B.15}$$

The parallel transport operator  $U_a[\mathbf{n}]$  gauge transforms as usual:  $U_a'[\mathbf{n}] = g[\mathbf{n} + \hat{a}]U_a[\mathbf{n}]g[\mathbf{n}]^{-1}$ , where  $g \in \mathbb{P}$ .

The 1-loop dynamics of the 5-vector must derive from a Lie-algebra-valued current  $\mathcal{J} \in \Lambda^1[\mathbb{Z}^4, \mathfrak{p}]$ . Since 1-loop theory forgoes a Hamiltonian or Lagrangian structure, the properties of this current must be independently defined. We therefore pause to define  $\mathcal{J}$  for a general lattice gauge theory in the 1-loop formalism.

**Definition:** Let  $G \rightarrow GL(V)$  be a representation of a Lie group  $G$  on a matter field  $\xi[\mathbf{n}] \in V$  valued in vector space  $V$ . Let  $\{\circ\!\!\!\circ\} = V \times V \times GL(V)$  denote the space of data determining a lattice edge in  $\mathbb{Z}^d$ . We define the *1-loop current*  $\mathcal{J} \in \Lambda^1[\mathbb{Z}^d, \mathfrak{g}]$  to be a  $G$ -equivariant  $\mathfrak{g}$ -valued 1-form, where  $\mathfrak{g} = \text{Lie}(G) \subset \mathfrak{gl}(V)$ . In particular,  $\mathcal{J} : \{\circ\!\!\!\circ\} \rightarrow \mathfrak{g}$  is required to satisfy  $\mathcal{J} \circ \Psi_g = \text{Ad}_g \circ \mathcal{J} \forall g \in G$ , where  $\Psi_g$

denotes the gauge transformation of a lattice edge, as follows:

$$\begin{aligned}\Psi_g : \{\circ\text{---}\circ\} &\rightarrow \{\circ\text{---}\circ\} \\ (\xi_1, \xi_2, U) &\mapsto (g \triangleright \xi_1, h \triangleright \xi_2, h \cdot U \cdot g^{-1})\end{aligned}\tag{B.16}$$

for  $h \in G$  arbitrary.

Thus, an arbitrary gauge transformation on  $\mathbb{Z}^4$  maps  $\mathcal{J}_a[\mathbf{n}]$  to

$$\mathcal{J}'_a[\mathbf{n}] = \mathcal{J}(\Psi_g(\mathfrak{z}_a)) = g[\mathbf{n}]\mathcal{J}_a[\mathbf{n}]g[\mathbf{n}]^{-1},\tag{B.17}$$

where  $\mathcal{J}_a[\mathbf{n}] = \mathcal{J}(\mathfrak{z}_a)$  and  $\mathfrak{z}_a = (\xi[\mathbf{n}], \xi[\mathbf{n} + \hat{a}], U_a[\mathbf{n}]) \in \{\circ\text{---}\circ\}$ . The preceding definition of the current thereby enforces an adjoint action befitting the red loop depicted in Fig. B.1.

This definition uniquely determines the  $\mathbb{1}$ -loop current of 5-vector lattice gauge theory. To see how, we first note that  $\mathcal{J}_a[\mathbf{n}]$  can only depend on  $\{\Phi[\mathbf{n}], \Phi[\mathbf{n} + \hat{a}], U_a[\mathbf{n}]\}$ . Furthermore, since the  $G$ -equivariance of  $\mathcal{J}_a[\mathbf{n}]$  precludes the appearance of  $g[\mathbf{n} + \hat{a}]$  in its gauge transformations, the dependence of  $\mathcal{J}_a[\mathbf{n}]$  on  $\{\Phi[\mathbf{n} + \hat{a}], U_a[\mathbf{n}]\}$  is limited to the pairing  $\Phi_a^+[\mathbf{n}] = U_a[\mathbf{n}]^{-1}\Phi[\mathbf{n} + \hat{a}]$ . (This construction accounts for the permissible arbitrariness of  $h$  in the definition of  $\Psi_g$  in Eq. (B.16).) We must therefore solve for a  $\mathfrak{p}$ -valued current  $\mathcal{J}_a[\mathbf{n}] = \mathcal{J}(\Phi, \Phi_a^+)$  that transforms in the adjoint Poincaré representation—that is

$$\begin{aligned}\text{Ad}_{(\Lambda, \varphi)} \begin{bmatrix} \Gamma & \mathbf{0} \\ e & 0 \end{bmatrix} &= \begin{bmatrix} \Lambda & \mathbf{0} \\ \varphi & 1 \end{bmatrix} \begin{bmatrix} \Gamma & \mathbf{0} \\ e & 0 \end{bmatrix} \begin{bmatrix} \Lambda & \mathbf{0} \\ \varphi & 1 \end{bmatrix}^{-1} \\ &= \begin{bmatrix} \Lambda\Gamma\Lambda^{-1} & \mathbf{0} \\ (\varphi\Gamma + e)\Lambda^{-1} & 0 \end{bmatrix}.\end{aligned}\tag{B.18}$$

Studying the Poincaré transformation of  $\Phi$  in Eq. (B.13), up to a multiplicative

constant there is found to be a unique such current:

$$\begin{aligned} \mathcal{J}_a[\mathbf{n}] &= \left[ \begin{array}{c|c} L^\mu_{\nu a}[\mathbf{n}] & \mathbf{0} \\ \hline T_{\nu a}[\mathbf{n}] & 0 \end{array} \right] \\ &= \frac{1}{2} \left[ \begin{array}{c|c} \pi^\mu \boxtimes (\pi_a^+)_\nu & \mathbf{0} \\ \hline \pi_\nu \phi_a^+ - \phi(\pi_a^+)_\nu & 0 \end{array} \right]. \end{aligned} \quad (\text{B.19})$$

Here,  $\pi_\nu = \pi^\sigma \eta_{\sigma\nu}$  and  $\boxtimes : \mathfrak{t}^* \times \mathfrak{t} \rightarrow \mathfrak{h}$  is the box map

$$x^\mu \boxtimes y_\nu = x \boxtimes (y^T \eta) = \left[ yx^T - xy^T \right] \eta, \quad (\text{B.20})$$

where  $\eta$  denotes the  $4 \times 4$  Minkowski matrix. ( $\boxtimes$  roughly resembles the hat map of a 4-vector cross product.) It is readily confirmed that under the gauge transformation of Eq. (B.13),  $\mathcal{J}_a[\mathbf{n}]$  transforms in the adjoint representation of Eq. (B.18), that is,  $\mathcal{J} \circ \Psi_g = \text{Ad}_g \circ \mathcal{J}$  holds.

We note that  $D_a^+ \Phi$  can be freely substituted for  $\Phi_a^+$  in Eq. (B.19) without affecting its value. In particular,  $L^\mu_{\nu a} = \frac{1}{2} \pi^\mu \boxtimes D_a^+ \pi_\nu$  since  $\pi^\mu \boxtimes \pi_\nu = 0$ , and  $T_{\nu a} = \frac{1}{2} (\pi_\nu D_a^+ \phi - \phi D_a^+ \pi_\nu)$  by a simple cancellation. In this form,  $T_{\nu a}$  more closely resembles a current equivalent to the energy-momentum  $T_{\mu\nu}^\phi$  of scalar field theory, as we now show.

We recall the two relations that define equivalence classes of nontrivial Noether currents in Lagrangian mechanics [53]. Two currents  $j_\mu[\phi] \cong \tilde{j}_\mu[\phi]$  are equivalent (in the sense that their mutual conservation arises from the same Noether symmetry) if they

- (i) differ by an expression that vanishes on-shell; or
- (ii) satisfy  $\partial^\mu (j_\mu[\phi] - \tilde{j}_\mu[\phi]) = 0$  off-shell.

We use both of these relations in the following calculation:

$$\begin{aligned}
T_{\mu\nu}^\phi &= \partial_\mu\phi\partial_\nu\phi - \frac{1}{2}\eta_{\mu\nu}(\partial^\sigma\phi\partial_\sigma\phi + m^2\phi^2) \\
&\stackrel{(i)}{\cong} \partial_\mu\phi\partial_\nu\phi - \frac{1}{2}\eta_{\mu\nu}(\partial^\sigma\phi\partial_\sigma\phi + \phi\partial^2\phi) \\
&\stackrel{(ii)}{\cong} \frac{1}{2}\left[\partial_\mu\phi\partial_\nu\phi - \phi\partial_\mu\partial_\nu\phi\right] \\
&\approx \frac{1}{2}e_\mu^a\left[\pi_\nu\partial_a\phi - \phi\partial_a\pi_\nu\right] \approx e_\mu^a T_{\nu a}|_{\mathbb{R}^{3,1}}
\end{aligned} \tag{B.21}$$

where we define  $T_{\nu a}|_{\mathbb{R}^{3,1}} = \frac{1}{2}(\pi_\nu\partial_a\phi - \phi\partial_a\pi_\nu)$ , and set  $\partial_\mu \approx e_\mu^a\partial_a$  and  $\pi_\nu \approx \partial_\nu\phi$  in the continuous, flat spacetime limit, as in [47, 48]. Therefore,  $T_{\nu a}|_{\mathbb{R}^{3,1}}$  forms a continuous analogue of the 5-vector energy-momentum  $T_{\nu a} = \frac{1}{2}(\pi_\nu D_a^+\phi - \phi D_a^+\pi_\nu)$ .

We now take up our central effort: the construction of  $\mathbb{P}$ -valued  $\mathbb{1}$ -loops that recover  $\delta DA + j = 0$  and  $\delta j = 0$  in the continuum limit. In Eq. (B.19), we have already derived a group-valued current suitable for the matter field sector of such  $\mathbb{1}$ -loops. In particular, we define  $J : \{\circ\text{--}\circ\} \rightarrow \mathbb{P}$  such that

$$J(\mathfrak{B}^{\circ\text{--}\circ}) = \exp(\kappa\mathcal{J}_a[\mathbf{n}]) \tag{B.22}$$

for some coupling constant  $\kappa$ . The first step in building the gauge field sector is similarly immediate: A realization of  $DA$  suitable for  $\mathbb{1}$ -loop theory is found at once in the Wilson loop, a 2-form  $\Omega : \{\square\} \rightarrow \mathbb{P}$  defined by  $\Omega(\mathfrak{B}^{\square}) = U_{ab}[\mathbf{n}]$ , as specified in Eq. (B.10).

To complete this construction, we must define a  $\mathbb{1}$ -loop covariant codifferential operator  $\delta$  and thereby assemble the desired  $\mathbb{P}$ -valued analogue of the Yang-Mills field equation,  $\delta\Omega \cdot J = \mathbb{1}$ . We require  $\delta$  to satisfy  $\delta^2\Omega = \mathbb{1}$  and  $(\delta\alpha)^{-1} = \delta(\alpha^{-1})$  for any form  $\alpha$ . The resulting  $\mathbb{1}$ -loop,  $\delta J = \mathbb{1}$ , will constitute a conservation law that determines matter field dynamics, as anticipated in Eq. (B.12). Taken together, these relations ensure the integrability (or solvability) of  $\mathbb{1}$ -loop theory.

It is illuminating to first consider what a  $\mathbb{1}$ -loop conservation law  $\delta J = \mathbb{1}$  could

look like. We assume that it holds at each  $\mathbf{n} \in \mathbb{Z}^4$ , so that currents along all eight lattice links terminating on  $\mathbf{n}$  ought to play a role. Whereas  $\mathcal{J}_a[\mathbf{n}]$  has endpoints at  $\mathbf{n}$ , however,  $\mathcal{J}_a[\mathbf{n} - \hat{a}]$  has endpoints at  $\mathbf{n} - \hat{a}$ . To incorporate the link  $[\mathbf{n} - \hat{a}|\mathbf{n}]$ , therefore, we substitute  $\Phi_a^+ \rightarrow \Phi_a^-$  in Eq. (B.19), yielding the  $\mathbf{p}$ -valued current  $\mathcal{J}_{\bar{a}}[\mathbf{n}]$ , defined as follows:

$$\mathcal{J}_{\bar{a}}[\mathbf{n}] = \mathcal{J}_a[\mathbf{n}] \Big|_{\Phi_a^+ \rightarrow \Phi_a^-} = -\text{Ad}_{U_a[\mathbf{n}-\hat{a}]} \mathcal{J}_a[\mathbf{n} - \hat{a}]. \quad (\text{B.23})$$

The currents  $\mathcal{J}_a[\mathbf{n} - \hat{a}]$  and  $\mathcal{J}_{\bar{a}}[\mathbf{n}]$  are defined by the same data,  $\omega_{\mathcal{B}} = (\Phi[\mathbf{n} - \hat{a}], \Phi[\mathbf{n}], U_a[\mathbf{n} - \hat{a}])$ . Their adjoint relationship in Eq. (B.23), readily confirmed using  $\Phi_a^-$  in Eq. (B.19), demonstrates their compatibility under parallel transport. Eq. (B.23) notably resembles the transformation of the Maurer-Cartan form  $\omega_G$  under the inversion map  $\iota$  [43]:  $(\iota^* \omega_G)(X_g) = -\text{Ad}_g(\omega_G(X_g)) \forall X_g \in T_g G$ .

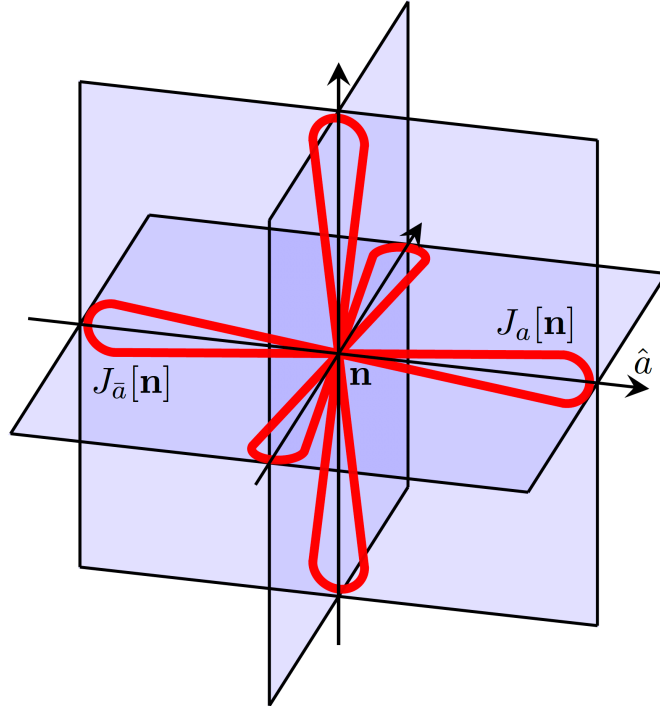


Figure B.2: Six of the eight elements comprising the  $\mathbb{1}$ -loop conservation law  $\delta J[\mathbf{n}] = [g_1 \cdots g_8](\mathcal{J}) = \mathbb{1}$  are depicted at vertex  $\mathbf{n}$ . In a continuous spacetime limit, this conservation law recovers its Yang-Mills analogue,  $\delta j = 0$ .

An intuitive  $\mathbb{1}$ -loop analogue for  $\delta j = 0$ , therefore, roughly takes the eight element form  $[g_1 \cdots g_8](\mathcal{J}) = \mathbb{1}$ , as depicted in Fig. B.2. The group elements  $\{g_i\}$  must depend on  $\mathcal{J}$  in a manner we shall make precise. To that end, we next revisit elements of Cartan geometry [43] and reinterpret them in the  $\mathbb{1}$ -loop formalism.

Let us recall  $\delta : \Lambda^\ell[M, \mathbb{R}] \rightarrow \Lambda^{\ell-1}[M, \mathbb{R}]$ , the codifferential of an  $\ell$ -form on a pseudo-Riemannian manifold  $M$ :

$$\delta\alpha = g^{ab}[\mathbf{i}_{e_a}(\nabla_{e_b}\alpha)] = \eta^{\mu\nu}[\mathbf{i}_{e_\mu}(\nabla_{e_\nu}\alpha)]. \quad (\text{B.24})$$

Here,  $\{e_a\}$  is any local basis of  $TM$  with inverse metric  $g^{ab}$  and  $\{e_\mu\}$  any local orthonormal basis.  $\mathbf{i}_X$  denotes an interior product and  $\nabla_X$  a covariant derivative with respect to  $X \in \mathfrak{X}(M)$ , where  $\mathfrak{X}(M) = \Gamma(TM)$  denotes the set of vector fields on  $M$ . Eq. (B.24) is equivalent to the more widely used definition,  $\delta = \pm\star d\star$  [132].

We now specialize  $M$  to spacetime, specifically, to the four-dimensional base space of a reductive Cartan geometry  $(P, \omega)$ . Here,  $\omega \in \Lambda^1[P, \mathfrak{p}]$  is a  $\mathfrak{p}$ -valued Cartan connection on the right  $H$ -principal bundle  $P \xrightarrow{\pi} M$ , where  $\mathfrak{p} = \mathfrak{h} \oplus \mathfrak{t}$  is a direct sum of  $\text{Ad}_H$ -modules and  $H = SO^+(3, 1)$ . A Cartan connection establishes, by definition, an isomorphism  $\omega_p : T_p P \rightarrow \mathfrak{p} \forall p \in P$ , such that  $\omega_p^{-1}$  is everywhere well-defined. As such, the universal covariant derivative with respect to  $A \in \mathfrak{p}$  of any function  $f \in \mathcal{C}(P)$  may be defined as follows [43]:

$$\nabla_A f = [\omega^{-1}(A)]f. \quad (\text{B.25})$$

$\nabla_A$  differentiates  $f$  with respect to the  $\omega$ -constant vector field  $\omega^{-1}(A) \in \mathfrak{X}(P)$ . In our notation, the universal  $\nabla_A$  is distinguished from  $\nabla_X$  merely by the distinct setting of  $A \in \mathfrak{p}$  and  $X \in \mathfrak{X}(M)$ .

An intuitive picture of this machinery will facilitate a  $\mathbb{1}$ -loop reformulation of  $\delta$ . First, we reinterpret the operator  $\nabla_{e_\mu}$  in Eq. (B.24) as the universal covariant

derivative of Eq. (B.25)—in particular, we regard  $e_\mu \in \mathfrak{t} \subset \mathfrak{p}$  as a Lie algebra element. For any such  $e_\mu \in \mathfrak{t}$ , the  $\omega$ -constant vector field  $\omega^{-1}(e_\mu)$  generates, by definition, geodesics on  $P$ .  $i_{e_\mu}(\nabla_{e_\mu}\alpha)$  therefore represents the change in  $\alpha$  along the geodesic generated by  $\omega^{-1}(e_\mu)$ .

In this way,  $\delta\alpha$  sums the change in  $\alpha$  over orthonormal geodesics, weighted by a metric factor as in Eq. (B.24). In the 1-loop formalism, this metric structure is not provided by the base manifold (or lattice) but by the Lie algebra  $\mathfrak{p}$ . In particular, we introduce the following nondegenerate,  $\text{Ad}_H$ -invariant metric  $\langle \cdot, \cdot \rangle_{\mathfrak{p}}$  on  $\mathfrak{p}$ :

$$\begin{aligned} \langle A, B \rangle_{\mathfrak{p}} &= \text{Tr}(A\boldsymbol{\eta}B^T\boldsymbol{\eta}) \quad \text{where } \boldsymbol{\eta} = \begin{bmatrix} \eta & \mathbf{0} \\ \mathbf{0} & 1 \end{bmatrix} \in \mathbb{R}^{5 \times 5} \\ &= \text{Tr}(\Gamma_A\boldsymbol{\eta}\Gamma_B^T\boldsymbol{\eta}) + e_A\boldsymbol{\eta}e_B^T \end{aligned} \quad (\text{B.26})$$

$\forall A, B \in \mathfrak{p}$ . Here,  $A = (\Gamma_A, e_A) \in \mathfrak{p}$  denotes a matrix Lie algebra element as appears in Eqs. (B.14) and (B.18), with  $e_A$  a row vector.  $e_A\boldsymbol{\eta}e_B^T$  may be recognized as the pseudo-Riemannian metric.

We now construct the 1-loop operator  $\delta$ . We first define a discrete Cartan connection  $\omega : \{\circ\text{-}\circ\} \rightarrow \mathfrak{p}$  such that  $\exp(\omega_a[\mathbf{n}]) = U_a[\mathbf{n}] \in \mathbb{P}$ . Since  $\delta$  aggregates over orthonormal geodesics, we choose an arbitrary basis  $\{e_\mu\}$  of  $\mathfrak{t} \subset \mathfrak{p}$  that is orthonormal with respect to  $\langle \cdot, \cdot \rangle_{\mathfrak{p}}$ . We further define the neighborhood  $\mathcal{N}_{\mathbf{n}}$  of  $\mathbf{n}$ , comprised of  $\mathbf{n}$  and its eight nearest neighbors in  $\mathbb{Z}^4$ . Now,  $\mathcal{N}_{\mathbf{n}}$  is said to be *rectified* if each connection  $\{\omega_a[\mathbf{n}], \omega_{\bar{a}}[\mathbf{n}]\}$  evaluates to a distinct basis vector in  $\{\pm e_\mu\}$ , e.g.  $\omega_x[\mathbf{n}] = -\omega_{\bar{x}}[\mathbf{n}] = e_\mu$ . To rectify  $\mathcal{N}_{\mathbf{n}}$ , we apply suitable gauge transformations at each neighbor of  $\mathbf{n}$ . We require, however, that the chosen transformations  $\{g[\mathbf{n} \pm \hat{a}] \in \mathbb{P}\}$  preserve the ‘isomorphism’ of  $\omega$  on  $\mathcal{N}_{\mathbf{n}}$ . In effect, the vierbeins  $e_a^\mu[\mathbf{n}]$  and  $e_{\bar{a}}^\mu[\mathbf{n}]$  should remain nonsingular as they are smoothly rectified toward  $(\pm)$  the identity matrix.

Concretely, this procedure yields transformed comparators of the form  $U'_a[\mathbf{n}] = g[\mathbf{n} + \hat{a}]U_a[\mathbf{n}] = \exp(e_\mu)$ , where  $g[\mathbf{n}] = \mathbb{1}$ . Any matter or gauge field data

that has already been defined within or adjoining  $\mathcal{N}_{\mathbf{n}}$  must also be gauge-transformed accordingly; therefore, not all lattice neighborhoods can be rectified simultaneously. We note that data as yet undefined need not (and of course cannot) be transformed in this way. We shall denote a rectified neighborhood by  $\bar{\mathcal{N}}_{\mathbf{n}}$ . Crucially, we observe that  $\bar{\mathcal{N}}_{\mathbf{n}}$  defines a bijection,  $r : \{\pm\mu\} \rightarrow \{a, \bar{a}\}$ .

At last, we define  $\delta : \Lambda^\ell[\bar{\mathcal{N}}_{\mathbf{n}}, \mathbb{P}] \rightarrow \Lambda^{\ell-1}[\bar{\mathcal{N}}_{\mathbf{n}}, \mathbb{P}]$  as a map between rectified  $\mathbb{P}$ -valued forms. A rectified form  $\alpha \in \Lambda^\ell[\bar{\mathcal{N}}_{\mathbf{n}}, \mathbb{P}]$  is a form defined on a rectified neighborhood that transforms under a gauge transformation as  $\alpha'[\mathbf{n}] = g[\mathbf{n}]\alpha[\mathbf{n}]g[\mathbf{n}]^{-1}$ . (Intuitively, a rectified form is a closed loop with endpoints at  $\mathbf{n}$ .) Clearly,  $J$  and  $\Omega$  are rectified forms on  $\bar{\mathcal{N}}_{\mathbf{n}}$ , while  $U_a = \exp(\omega_a)$  is not.  $\delta$  is now readily defined:

$$\begin{aligned}\delta J[\mathbf{n}] &= \exp \sum_{\nu \in \{\pm\mu\}} \log J^\nu[\mathbf{n}] \\ \delta \Omega_b[\mathbf{n}] &= \exp \sum_{\nu \in \{\pm\mu\}} \log \Omega_b^\nu[\mathbf{n}].\end{aligned}\tag{B.27}$$

The notation of Eq. (B.27) requires some clarification.  $\exp$  and  $\log$  denote matrix exponentials and logarithms, respectively. As in Eq. (B.10), a raised index indicates a metric factor, such that  $\log J^\mu = \eta^{\mu\mu} \log J_\mu$ . (This metric factor is now seen to arise from its associated  $e_\mu$  geodesic.) Furthermore,  $J_\mu[\mathbf{n}]$  denotes  $J_{r(\mu)}[\mathbf{n}]$ , the current on a single link in  $\bar{\mathcal{N}}_{\mathbf{n}}$ , as determined by the bijection  $r$ . Similarly,  $\Omega_{\mu b}[\mathbf{n}]$  denotes the holonomy  $\Omega_{r(\mu)b}[\mathbf{n}]$  on a single plaquette. As seen in Eq. (B.23), the ‘backward’ currents  $\{\mathcal{J}_{\bar{a}}\}$  are implicitly negated, as are the ‘reversed’ holonomies  $\{\log \Omega_{\bar{a}b}\}$ . Thus, the intuitive picture of  $\delta J$  (or  $\delta \Omega$ ) as the metric-weighted change in  $J$  (or  $\Omega$ ) along geodesics is realized.

The use of the logarithm in the definition of  $\delta$  enables the ‘simultaneous’ multiplication of non-abelian group elements—without preferential ordering.  $\delta$  of a rectified 1-form (e.g.  $\delta J$ ) can therefore be imagined as a simultaneous contraction of loops along all edges adjoining a vertex, and  $\delta$  of a rectified 2-form (e.g.  $\delta \Omega$ ) as the simul-

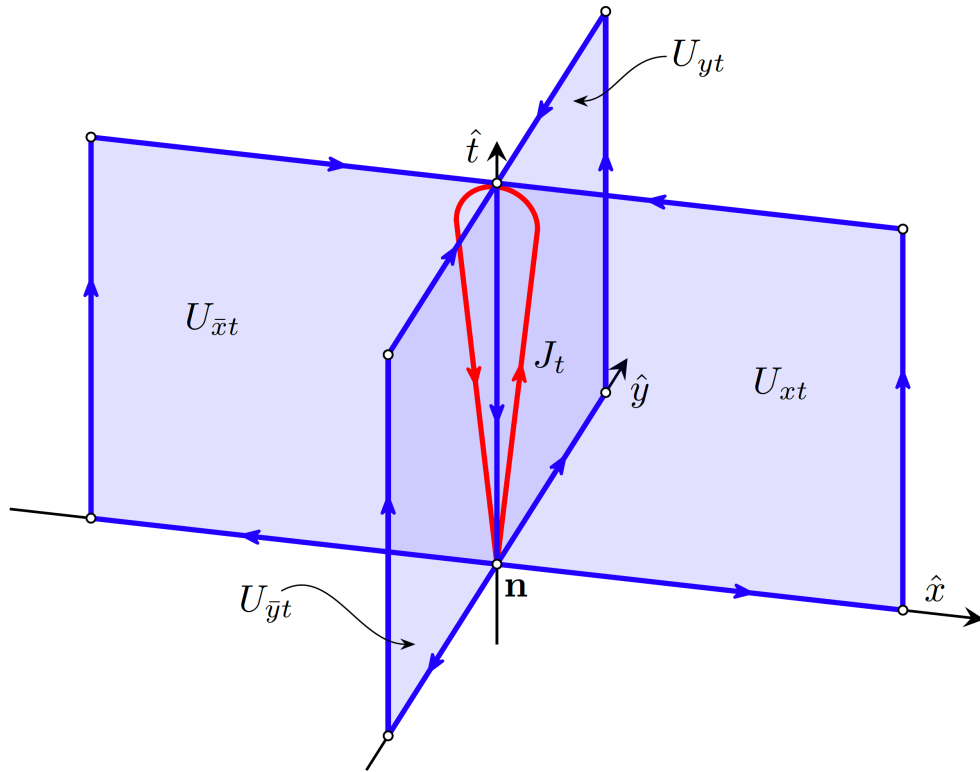


Figure B.3: Four of the six holonomies comprising the 1-loop  $\delta\Omega_t[\mathbf{n}]J_t[\mathbf{n}] = 1$  are depicted with  $J_t[\mathbf{n}]$ . ( $U_{zt}$  and  $U_{\bar{z}t}$  are not shown.)  $\delta\Omega_t[\mathbf{n}]$  can be regarded as a ‘simultaneous’ multiplication of the six holonomies adjoining lattice edge  $[\mathbf{n}|\mathbf{n} + \hat{t}]$ .

taneous contraction of loops along all plaquettes adjoining an edge. (See Figs. B.2 and B.3.) The absence of ordering in these multiplications ensures that  $\delta^2\Omega = \mathbb{1}$  and  $(\delta\alpha)^{-1} = \delta(\alpha^{-1})$ , properties of  $\delta$  that are readily verified with Eq. (B.27).

The basic  $\mathbb{1}$ -loop of Eq. (B.1) is now completely defined. Lattice fields are thus evolved by solving the  $\mathbb{1}$ -loops  $\delta\Omega_a \cdot J_a = \mathbb{1}$  and  $\delta J = \mathbb{1}$  for their unknown data. We assume that this evolution proceeds time-slice by time-slice, and is therefore realizable by the following iterative algorithm:

- (i) Self-consistently initialize  $\Phi[\mathbf{n}]$ ,  $\Phi[\mathbf{n} + \hat{t}]$ ,  $\omega_a[\mathbf{n}]$  and  $\omega_b[\mathbf{n} + \hat{t}] \forall \mathbf{n} \in \{n_t = 0\}$ ,  $a \in \{t, \mathbf{x}\}$  and  $b \in \{\mathbf{x}\}$ .
- (ii) Since no  $\mathbb{1}$ -loop is completed by defining a gauge field along a temporal link  $[n_t = 1 | n_t = 2]$ , any such link may be freely specified. Thus, assign the temporal gauge:  $\omega_t[\mathbf{n}] = e_0 \forall \mathbf{n} \in \{n_t = 1\}$ .
- (iii) Solve  $\delta J[\mathbf{n}] = \mathbb{1}$  for  $\Phi[\mathbf{n} + \hat{t}] \forall \mathbf{n} \in \{n_t = 1\}$ .
- (iv) Solve  $\delta\Omega_b[\mathbf{n}]J_b[\mathbf{n}] = \mathbb{1}$  for  $\omega_b[\mathbf{n} + \hat{t}] \forall \mathbf{n} \in \{n_t = 1\}$  and  $b \in \{\mathbf{x}\}$ .
- (v) Return to (ii), assigning  $\omega_t[\mathbf{n}] = e_0 \forall \mathbf{n} \in \{n_t = 2\}$ .

A conceptually straightforward approach to calculating  $\delta$  in steps (iii) and (iv) is to rectify a maximal set of disjoint neighborhoods  $\bar{\mathcal{M}} = \sqcup_{\mathbf{n}} \{\bar{\mathcal{N}}_{\mathbf{n}}\}$  on  $\mathbb{Z}^4|_{n_t=1}$ , solve for rectified forms on  $\bar{\mathcal{M}}$ , and then repeat for the as-yet-unrectified neighborhoods on  $\mathbb{Z}^4|_{n_t=1} \setminus \bar{\mathcal{M}}$ . We note, however, that rectified forms on a neighborhood  $\mathcal{N}_{\mathbf{n}}$  are in fact invariant under the ‘ $\mathbf{n}$ -adjacent’ transformations  $\{g[\mathbf{n} \pm \hat{a}]\}$  (since their loops terminate at  $\mathbf{n}$ ). In principle, therefore, a more streamlined approach could solve all neighborhoods of  $\mathbb{Z}^4$  in parallel as if they were rectified, and afterward resolve any mismatches of gauge. We observe that the preceding algorithm maximally leverages the gauge-invariance of the  $\mathbb{1}$ -loop; the rectification of  $\mathcal{N}_{\mathbf{n}}$  by  $\delta$  is made permissible by the gauge invariance of  $\delta J = \mathbb{1}$  and  $\delta\Omega_b[\mathbf{n}]J_b[\mathbf{n}] = \mathbb{1}$ .

Let us consider the solvability of this algorithm. A self-consistent initialization of step (i) requires that  $\delta\Omega_t[\mathbf{n}]J_t[\mathbf{n}] = \mathbb{1} \forall \mathbf{n} \in \{n_t = 0\}$ . By specifying  $J_t[\mathbf{n}] \in \mathbb{P}$  first, and then the matter fields  $\Phi[\mathbf{n}]$  and  $\Phi_t^+[\mathbf{n}]$  comprising it, various suitable initial conditions are readily found. All steps of the algorithm are then immediately solvable, except perhaps step (iii). We note, however, that Eq. (B.19) is linear in  $\Phi_a^+$ . Therefore, since every leg of  $\delta J[\mathbf{n}]$  shares the same  $\Phi[\mathbf{n}]$ , a solution  $\Phi_t^+[\mathbf{n}]$  to  $\delta J[\mathbf{n}] = \mathbb{1}$  must exist. For completeness, we nevertheless note the following conditions on  $\Phi = [\pi^\mu; \phi]$  necessary for the existence of a solution  $\Phi_t^+$  to  $\mathcal{J}(\Phi, \Phi_t^+) = (\Gamma^\mu_\nu, e_\nu)$ :

$$\begin{aligned} \pi^\mu \boxtimes e_\nu + \phi \Gamma^\mu_\nu &= 0 \\ \pi^\sigma \Gamma^{\tau\mu} + \pi^\tau \Gamma^{\mu\sigma} + \pi^\mu \Gamma^{\sigma\tau} &= 0, \end{aligned} \tag{B.28}$$

where  $(\Gamma^\mu_\nu, e_\nu) \in \mathfrak{p}$  and  $\Gamma^{\sigma\tau} = \Gamma^\sigma_\nu \eta^{\nu\tau}$ .

Furthermore, when the representation  $\Phi$  is fully specified, the preceding algorithm is not only solvable but uniquely determined—up to arbitrary choices of gauge. In particular, once the mass and ‘time direction’ of  $\Phi$  are fixed (such that  $\pi^\mu \pi_\mu + m^2 = 0$  and  $\pi^0 > 0 \forall \mathbf{n}$ , for example), the conservation law  $\delta J = \mathbb{1}$  fully determines its evolution. Likewise,  $\delta\Omega \cdot J = \mathbb{1}$  uniquely determines  $\omega_a$ .

We shall leave a more robust examination of the dynamics of  $\Phi$  to future work. For now, having described an algorithm for the evolution of Poincaré 1-loop theory, we examine its physics in the continuum limit.

## B.5 Gravity in the 1-loop Formalism

We consider the continuum limit of 1-loop Poincaré lattice gauge theory. We denote our gauge field by  $\omega_a[\mathbf{n}] = A_a[\mathbf{n}] \in \mathfrak{p}$  and define its comparators with a lattice parameter  $\Delta$ , that is:  $U_a[\mathbf{n}] = \exp(\Delta A_a[\mathbf{n}])$ . Applying the BCH formula—see [133] Eq. (8.7)—and expanding gauge fields at lattice points away from  $\mathbf{n}$ —e.g.

$A_b[\mathbf{n} \pm \hat{a}] = [A_b \pm \Delta \partial_a A_b + \frac{\Delta^2}{2} \partial_a^2 A_b + \mathcal{O}(\Delta^3)]$ —we find, in the  $\Delta \rightarrow 0$  limit:

$$\log U_{ab}[\mathbf{n}] = \Delta^2 F_{ab} + \mathcal{O}(\Delta^3) \quad (\text{B.29})$$

$$\log U_{\hat{a}b}[\mathbf{n}] + \log U_{ab}[\mathbf{n}] = \Delta^3 D_a F_{ab} + \mathcal{O}(\Delta^4),$$

where  $F_{ab} = \partial_{[a} A_{b]} - [A_a, A_b]$  and  $D_a = \partial_a - [A_a, \cdot]$ . (Note, no index summation is implied in Eq. (B.29); we omit the conventional factor of  $\frac{1}{2}$  in our notation for the antisymmetrization of indices; and the sign conventions in  $F_{ab}$  and  $D_a$  arise because the gauge field has a left action,  $\triangleright$ .) Computing the Lie brackets in the definitions of  $F_{ab}$  and  $D_a$ , we explicitly evaluate the fields of Eq. (B.29) for our  $\mathfrak{p}$ -valued connection as follows:

$$A_a = \left[ \begin{array}{c|c} \Gamma^\mu_{\nu a} & \mathbf{0} \\ \hline e_{\nu a} & 0 \end{array} \right] \quad (\text{B.30a})$$

$$F_{ab} = \left[ \begin{array}{c|c} F^\mu_{\nu ab} & \mathbf{0} \\ \hline F_{\nu ab} & 0 \end{array} \right] = \left[ \begin{array}{c|c} \partial_{[a} \Gamma^\mu_{\nu|b]} - \Gamma^\mu_{\sigma[a} \Gamma^\sigma_{\nu|b]} & \mathbf{0} \\ \hline \partial_{[a} e_{\nu|b]} - e_{\sigma[a} \Gamma^\sigma_{\nu|b]} & 0 \end{array} \right] \quad (\text{B.30b})$$

$$D_c F_{ab} = \left[ \begin{array}{c|c} \partial_c F^\mu_{\nu ab} - \Gamma^\mu_{\sigma c} F^\sigma_{\nu ab} + F^\mu_{\sigma ab} \Gamma^\sigma_{\nu c} & \mathbf{0} \\ \hline \partial_c F_{\nu ab} - e_{\sigma c} F^\sigma_{\nu ab} + F_{\sigma ab} \Gamma^\sigma_{\nu c} & 0 \end{array} \right]. \quad (\text{B.30c})$$

We now substitute Eqs. (B.27), (B.29) and (B.30c) into the 1-loop  $\delta\Omega_b[\mathbf{n}] J_b[\mathbf{n}] = \mathbb{1}$  of Eq. (B.1), keeping terms to least order in  $\Delta$ . Working on  $\bar{\mathcal{N}}_{\mathbf{n}}$ , we thus discover

$$D^a F_{ab} + \kappa \mathcal{J}_b = \left[ \begin{array}{c|c} \partial^a F^\mu_{\nu ab} + \kappa L^\mu_{\nu b} & \mathbf{0} \\ \hline \partial^a F_{\nu ab} - e_\sigma^a F^\sigma_{\nu ab} + \kappa T_{\nu b} & 0 \end{array} \right] = 0, \quad (\text{B.31})$$

where we have set  $\Gamma^\mu_{\nu a}[\mathbf{n}] = 0$  and  $g^{ab}[\mathbf{n}] = \eta^{ab}$ . (In the continuum limit, rectification resembles a local application of Riemann normal coordinates.)  $L^\mu_{\nu b}$  and  $T_{\nu b}$  in Eq. (B.31) are assumed to be in the  $\Delta \rightarrow 0$  limit. Restoring  $\Gamma^\mu_{\nu a}$ , we may re-express

the field equations of Eq. (B.31) more schematically as

$$\begin{aligned}\partial R - [\Gamma, R] + \kappa L &= 0 \\ \partial S - [e, R] - [\Gamma, S] + \kappa T &= 0\end{aligned}\tag{B.32}$$

where  $R$  (i.e.  $F^\mu_{\nu ab}$ ) and  $S$  (i.e.  $F_{\nu ab}$ ) roughly represent spacetime curvature and torsion, respectively—an interpretation we shall justify in Eq. (B.36). We emphasize that these field equations comprise the continuous limit of the well-posed discrete algorithm of the previous section.

Let us compare this result with existing gauge theories of gravity. The earliest attempt at a modern gauge theory of gravity was made in 1955 by Utiyama [134], who identified the Lorentz group as the relevant gauge group.  $SO^+(3, 1)$  is an instinctive fit for gravity, not least because the Lorentz field strength  $F^\mu_{\nu ab}$  essentially reproduces the Riemann tensor of curved spacetime, as in Eq. (B.36). Utiyama’s formalism appears to suggest [135], however, that the sole Noether current associated with gravity is angular momentum ( $L$ )—a result that perhaps underrates energy-momentum ( $T$ ) as a source of gravitation.

Subsequent efforts were made to incorporate a more complete description of the gauge symmetries and conserved quantities of gravity. An examination of the literature reveals that, since the 1960s, at least two parallel tracks developed in Poincaré gauge theories of gravity. These might be called the L (Lagrangian) track [115–121] and the YM (Yang-Mills) track [122–127].

The widely studied L-track originated in the 1960s. Kibble [115] and Sciama [116] extended Utiyama’s gauge theory to the Poincaré group, yielding Einstein-Cartan-Sciama-Kibble gravity, or  $U_4$  theory [117–120]. While the Poincaré gauge field curvatures of  $U_4$  theory are identical to those of Eq. (B.30b), the matter couplings of its field equations differ considerably from those of Eq. (B.32). In its simplest form,  $U_4$  theory couples angular momentum ( $L$ ) not with curvature ( $R$ ), but with a non-propagating

torsion ( $S$ ). Somewhat unexpectedly, therefore, angular momentum is coupled in  $U_4$  theory to the gauge field curvature associated with the translation subgroup  $\mathbb{T}^{3,1} \subset \mathbb{P}$ . The L-track hews to a Lagrangian formalism and, in all of its manifestations, derives from the *terra firma* of a variational principle. Lattice reformulations of the L-track have also been widely explored [136–142].

The YM-track originated in the 1970s with an attempt by Popov and Daikhin [122, 123] to derive a more orthodox gauge theory of gravitation. This branch of Poincaré gauge theory is of particular relevance here, because its field equations [124, 125] are precisely recovered in the continuum limit of Poincaré  $\mathbb{1}$ -loop theory, as derived in Eqs. (B.31)-(B.32). Unlike those of the L-track, these field equations couple a propagating torsion ( $\partial S$ ) to energy-momentum ( $T$ ). The YM-track has proven to be underivable from a Lagrangian formalism [124–127]. It is perhaps unsurprising, then, that a new dynamical formalism such as  $\mathbb{1}$ -loop theory might, in its continuum limit, rediscover it. We shall further characterize key results of the YM-track in our concluding discussion. For now, having contextualized the continuum limit of Poincaré  $\mathbb{1}$ -loop theory, we proceed to demonstrate its recovery of Einstein’s vacuum equations.

We take a general relativistic (GR) limit of Eq. (B.31) by imposing two additional assumptions upon it, namely, metric compatibility and zero torsion. The former— $D_c g_{ab} = 0$ —may be established by defining a vanishing covariant derivative of the translation gauge field [143]:

$$\begin{aligned} 0 &= D_a e_{\mu b} \\ &= \partial_a e_{\mu b} + \Gamma_{\mu a}^{\sigma} e_{\sigma b} + \Gamma_{ba}^c e_{\mu c}. \end{aligned} \tag{B.33}$$

Here, we have introduced the affine connection  $\Gamma_{ba}^c$ , whose degrees of freedom are not independent and are fixed in terms of the Poincaré gauge fields by Eq. (B.33). The

Riemann tensor is then defined as usual in terms of this affine connection:

$$R^c{}_{dab} = \partial_{[a}\Gamma^c{}_{d|b]} - \Gamma^c{}_{e[a}\Gamma^e{}_{d|b]}. \quad (\text{B.34})$$

The latter assumption, zero torsion, is defined as follows:

$$S^c{}_{ab} = \Gamma^c{}_{[ab]} = 0. \quad (\text{B.35})$$

We now substitute Eqs. (B.33)-(B.35) to eliminate the Lorentz gauge field  $\Gamma^\mu{}_{\nu a}$  in Eq. (B.30b). Simplifying, we find that in the GR limit

$$\begin{aligned} F^\mu{}_{\nu ab} &= e^{\mu d} e_{\nu c} R^c{}_{dba} \\ F_{\nu ab} &= e_{\nu c} S^c{}_{ab} = 0, \end{aligned} \quad (\text{B.36})$$

where  $e^\mu{}_b e_\mu{}^a = \delta_b^a$  and  $g_{ab} = e^\mu{}_a \eta_{\mu\nu} e^\nu{}_b$ . Therefore, the Riemann and torsion tensors are closely related to the gauge field curvatures defined in Eq. (B.30b), as desired. Since  $F^{\mu\nu}{}_{ab}$  is antisymmetric in its first two and last two indices, it further follows from Eq. (B.36) that, in the GR limit,  $R^{cd}{}_{ab}$  is as well.

Finally, substituting Eq. (B.36) into the translation components of Eq. (B.31) and setting  $T_{\nu b} = 0$ , we thus recover Einstein's vacuum equations

$$e_{\nu c} R^{ca}{}_{ba} = 0, \quad (\text{B.37})$$

as desired.

## B.6 Discussion and Conclusions

The  $\mathbb{1}$ -loop formalism has been demonstrated to successfully define a lattice gauge theory of the Poincaré group. By reinterpreting  $\mathbb{P}$  as an internal gauge group,  $\mathbb{1}$ -loop

theory describes Poincaré symmetry on a discrete lattice, and recovers Einstein’s vacuum equations in its torsionless, continuum vacuum limit. This new formalism comprises several technical innovations:

- (i) the  $\mathbb{1}$ -loop of Eq. (B.4)—a relative of the Wilson loop that reconstitutes differential equations of motion;
- (ii) the 5-vector  $\Phi$  of Eq. (B.13)—a new representation of the Poincaré group;
- (iii) the definition of  $\mathbb{1}$ -loop current, which uniquely determines the Poincaré current  $\mathcal{J}_a$  of Eq. (B.19); and
- (iv) the lattice covariant codifferential  $\delta$  of Eq. (B.27), motivated by Cartan geometry.

The dynamics of the resulting Poincaré gauge theory are determined by the basic  $\mathbb{1}$ -loop  $\delta\Omega \cdot J = \mathbb{1}$ , as defined in Eq. (B.1). This  $\mathbb{P}$ -valued analogue of a Yang-Mills field equation defines not only the dynamics of the Poincaré gauge field, but matter field dynamics as well. Indeed, matter field equations of motion are superfluous in  $\mathbb{1}$ -loop theory, as they follow from the conservation of the  $\mathbb{P}$ -valued Noether current,  $\delta J = \mathbb{1}$ , guaranteed in turn by  $\delta^2\Omega = \mathbb{1}$ . The  $\mathbb{1}$ -loop formalism thereby defines a computable, exactly-energy-momentum-conserving algorithm for the dynamics of a 5-vector matter field evolving under gravity.

A  $\mathbb{1}$ -loop theory is decidedly rigid in the sense that very few arbitrary choices are made in its construction. Given a  $G$ -representation and a reductive Cartan geometry with  $\mathfrak{g}$ -valued connection  $\omega$  and base-space  $M$ , a corresponding  $\mathbb{1}$ -loop theory is already quite fixed: the hypercubic lattice  $\mathbb{Z}^d$  is defined such that  $d = \dim[M]$ ; the holonomy  $\Omega$  is fixed by  $\omega$ ; the  $\mathbb{1}$ -loop current  $J$  is fixed by the  $G$ -representation, as demonstrated for  $G = \mathbb{P}$  in Eq. (B.19); and the interaction of matter and gauge fields is wholly determined by the  $\mathbb{1}$ -loop  $\delta\Omega \cdot J = \mathbb{1}$ . The definition of the operator  $\delta$  is itself quite constrained by its need to satisfy  $\delta^2\Omega = \mathbb{1}$ .

Nevertheless, the status of Poincaré symmetry with respect to  $\delta$  is not clear. An ‘external’ Lorentz metric,  $\eta^{\mu\nu}$  is applied in Eq. (B.27) in such a way that the mixed Lorentz signature is identified with edges of the lattice. So while this data should be exclusively the result of the gauge fields themselves, an external metric nevertheless enters the theory.

The choice to relinquish a Lagrangian in favor of the  $\mathbb{1}$ -loop formalism was not undertaken without considerable effort by the authors to construct a satisfactory Lagrangian Poincaré lattice gauge theory. However, in a Lagrangian approach, Poincaré symmetry generators naturally arise as vector fields on spacetime, which are ill-defined on a discrete lattice. An effort to ‘lift’ these generators to vertical gauge symmetries of a discrete Lagrangian apparently requires the introduction of new fields that do not have a clear physical interpretation [47, 48]. More abstractly, this earlier work revealed a natural tension between the additive structure of a Lagrangian action—integrated over spacetime or summed over lattice vertices—and the multiplicative group structure of the Poincaré symmetries.

A Hamiltonian approach was also considered, however, operator-based Hamiltonian theories are predicated on the evolution of a continuous time parameter that is unsuitable for computation. Although gauge-compatible splitting methods [19] enable the preservation of gauge structure in discrete-time Hamiltonian algorithms, it is unclear how such a splitting in time can be extended to a ‘four-dimensional splitting’ over a spacetime lattice.

The  $\mathbb{1}$ -loop formalism was developed to address these challenges. It assumes a multiplicative structure on the lattice, wherein adjacent vertices are related strictly by group-valued fields. The result can be viewed as a discrete realization of the integral formalism [144] of early gauge theory.

The continuum limit of  $\mathbb{1}$ -loop theory, as derived in Eqs. (B.31)-(B.32), recovers the field equations of the YM-track of Poincaré gauge theory [122–127]. Despite

the YM-track exhibiting many promising features of a gravitational theory [125], the incompatibility of its field equations with Lagrangian mechanics has led some of its investigators to view the YM-track with disfavor [124, 126, 127]. Poincaré 1-loop theory addresses some of the concerns raised in this prior work, as we now discuss.

First, the determination of matter couplings in the YM-track has not been well understood; for example, the interpretation of  $T$  in Eq. (B.32) as an energy-momentum has been in doubt [124]. 1-loop theory addresses this issue by defining a new formalism that explicitly defines the properties of a matter current and its coupling to a gauge field. In Eq. (B.19), this formalism was shown to uniquely determine  $\mathcal{J}_a$ , the  $\mathfrak{p}$ -valued current of the 5-vector field. Second, from a more philosophical point of view, authors of the YM-track caution generally against its failure to derive from a variational principle [124, 126]. However, the crucial use of Cartan geodesics in the 1-loop formalism lends it a variational character, even absent a Lagrangian.

Lastly, some authors of the YM-track note that, although it has not made unphysical predictions of classical gravitational dynamics, its lack of a Lagrangian complicates its quantization via a path integral approach. This difficulty is understood to render the YM-track unsuitable as a quantum theory of gravity [127].

# Appendix C

## Toward the inclusion of $U(1)$ in $\mathbb{1}$ -loop theory

### C.1 Introduction

In Appendix B, a lattice gauge theory was constructed from a new non-unitary, irreducible representation of the Poincaré group  $\mathbb{P}$ , adapted from the Bargmann representation of spacetime transformations. Instead of defining spacetime as the target space of  $\mathbb{P}$ , the new representation acted upon a finite-dimensional matter field called a *5-vector* at each lattice vertex. The  *$\mathbb{1}$ -loop formalism* was constructed to define the dynamics of this 5-vector—and the gravitational Poincaré gauge field—on the lattice. The original motivation for such a theory was a desire to define a Poincaré-invariant physical theory suitable for computer simulation—an endeavor that necessitated a reinterpretation of Poincaré symmetry as an internal gauge symmetry.

A parallel effort is undertaken in the present appendix to define a  $\mathbb{1}$ -loop theory for a spinful Poincaré representation. Unlike our previous study—which required the discovery of the 5-vector representation—a spinful field suitable for  $\mathbb{1}$ -loop theory has already appeared in the literature: the twistor [145]. Whereas the 5-vector naturally

induces a 1-loop theory with gauge group  $\mathbb{P}$ , however, the natural gauge group of a 1-loop theory for the twistor is found to be the 16-dimensional pseudo-unitary group  $U(2, 2)$ .

Penrose devised the twistor as a representation of a complexified, compactified Minkowski spacetime. Following the 1-loop formalism, however, we treat the twistor as a matter field on the lattice—a ‘completion’ of sorts of the Dirac fermion. In particular, while Dirac’s 4-component spinor is defined by its Lorentz transformations, Penrose’s 4-component twistor is defined to transform under the 15-dimensional conformal group,  $\mathbf{conf}(\mathbb{R}^{3,1}) \cong SU(2, 2)$ . In the 1-loop formalism, the central extension  $U(2, 2) \cong SU(2, 2) \times U(1)$  appears as the natural transformation group of the twistor.

## C.2 The 5-Vector Representation of $\mathfrak{p}$

### C.2.1 The representation and matter field

To review, the 5-vector representation  $\rho_5 : \mathfrak{p} \rightarrow \mathfrak{gl}_5(\mathbb{R})$  of the Poincaré Lie algebra  $\mathfrak{p} = \mathbf{Lie}(\mathbb{P})$  is defined as follows:

$$[P^\alpha]^\mu{}_\sigma := \begin{bmatrix} \mathbb{0} & \mathbf{0} \\ \delta_\sigma^\alpha & 0 \end{bmatrix} \quad [M^{\alpha\beta}]^\mu{}_\sigma := \left[ \begin{array}{c|c} \eta^{\alpha\mu}\delta_\sigma^\beta - \eta^{\beta\mu}\delta_\sigma^\alpha & \mathbf{0} \\ \hline \mathbf{0} & 0 \end{array} \right]. \quad (\text{C.1})$$

It is readily checked that Eq. (C.1) satisfies the Lie algebra of spacetime symmetry generators  $P^\alpha = \partial^\alpha$  and  $M^{\alpha\beta} = x^\alpha \partial^\beta - x^\beta \partial^\alpha$ :

$$\begin{aligned} [P^\alpha, P^\beta] &= 0 \\ [M^{\alpha\beta}, M^{\mu\nu}] &= \eta^{\beta\mu} M^{\alpha\nu} + \eta^{\alpha\nu} M^{\beta\mu} - \eta^{\alpha\mu} M^{\beta\nu} - \eta^{\beta\nu} M^{\alpha\mu} \\ [M^{\alpha\beta}, P^\mu] &= \eta^{\beta\mu} P^\alpha - \eta^{\alpha\mu} P^\beta. \end{aligned} \quad (\text{C.2})$$

Let us denote  $\rho_5(\mathbb{P}) = \exp[\rho_5(\mathfrak{p})]$ . At any lattice vertex  $\mathbf{n} \in \mathbb{Z}^4$ , the 5-vector  $\Phi[\mathbf{n}]$  is then defined to transform under the left action  $\triangleright$  of  $g \in \rho_5(\mathbb{P})$  as follows:

$$g \triangleright \Phi[\mathbf{n}] = \begin{bmatrix} \Lambda^\mu{}_\nu & 0 \\ \varphi_\nu & 1 \end{bmatrix} \cdot \begin{bmatrix} \pi^\nu[\mathbf{n}] \\ \phi[\mathbf{n}] \end{bmatrix} = \begin{bmatrix} \Lambda^\mu{}_\nu \pi^\nu[\mathbf{n}] \\ \phi[\mathbf{n}] + \varphi_\nu \pi^\nu[\mathbf{n}] \end{bmatrix}. \quad (\text{C.3})$$

Eq. (C.1) is, therefore, an irreducible representation of  $\mathfrak{p}$  on the real vector space of 5-vectors  $\{\Phi\}$ , a spin-0 matter field roughly analogous to a scalar field in spacetime. A local gauge transformation  $\Psi_g$  specifies  $g[\mathbf{n}] \in \rho_5(\mathbb{P}) \forall \mathbf{n} \in \mathbb{Z}^4$ .

### C.2.2 The 1-loop current

In Appendix B, dynamics were defined for the field  $\Phi$  on  $\mathbb{Z}^4$  by means of the identity-valued 1-loop

$$\delta\Omega \cdot J = \mathbb{1}, \quad (\text{C.4})$$

where  $\Omega_{ab}[\mathbf{n}] \in \rho_5(\mathbb{P})$  denotes a group-valued Wilson loop based at  $\mathbf{n}$ , and  $J_a[\mathbf{n}] = \exp(\mathcal{J}_a[\mathbf{n}]) \in \rho_5(\mathbb{P})$  was defined by the 1-loop current  $\mathcal{J}_a[\mathbf{n}]$  (see Eq. (B.19)) along lattice edge  $[\mathbf{n}|\mathbf{n} + \hat{a}]$  as follows:

$$\mathcal{J}_a[\mathbf{n}] = \frac{1}{2} \left( \Phi(\Phi_a^+)^T - \Phi_a^+ \Phi^T \right) \eta_0. \quad (\text{C.5})$$

Here,  $\Phi_a^+[\mathbf{n}] = U_a[\mathbf{n}]^{-1} \Phi[\mathbf{n} + \hat{a}]$  denotes a neighboring 5-vector, pulled back by the  $\rho_5(\mathbb{P})$ -valued comparator  $U_a[\mathbf{n}]$ , and  $\eta_0 = \mathbf{diag}(-1, 1, 1, 1, 0)$ . The argument  $[\mathbf{n}]$  of a field defined at  $\mathbf{n}$  will often be suppressed as in Eq. (C.5).

It is readily checked that  $\mathcal{J}_a[\mathbf{n}]$  of Eq. (C.5) satisfies the defining properties of a 1-loop current for the representation  $\rho_5(\mathfrak{p})$ :

- (i)  $\mathcal{J}_a[\mathbf{n}]$  is  $\rho_5(\mathfrak{p})$ -valued;

- (ii)  $\mathcal{J}_a[\mathbf{n}]$  is a function of  $\Phi[\mathbf{n}]$  and  $\Phi_a^+[\mathbf{n}]$ ; and
- (iii) Under a local gauge transformation  $\Psi_g$  on  $\mathbb{Z}^4$  such that

$$\Phi'[\mathbf{n}] = \Psi_g(\Phi[\mathbf{n}]) = g[\mathbf{n}]\Phi[\mathbf{n}], \quad (\text{C.6})$$

$\mathcal{J}_a$  transforms adjointly, that is,  $\mathcal{J}'_a[\mathbf{n}] = g[\mathbf{n}]\mathcal{J}_a[\mathbf{n}]g[\mathbf{n}]^{-1}$ .

In particular, we note that  $g^T \eta_0 g = \eta_0 \forall g \in \rho_5(\mathbb{P})$ .

This adjoint transformation of  $\mathcal{J}_a$  encourages its interpretation as a loop formed along a lattice edge, and facilitates its concatenation with Wilson loops via group multiplication. Thus, with the aid of a covariant codifferential  $\delta$ , the identity-valued  $\mathbb{1}$ -loop  $\delta\Omega \cdot J = \mathbb{1}$  may be formed.

## C.3 The Twistor Representation of $\mathfrak{p}$

### C.3.1 The representation and matter field

Analogously, we now develop a spin- $\frac{1}{2}$  matter field representation suitable for  $\mathbb{1}$ -loop theory. In particular, we seek a finite-dimensional spin- $\frac{1}{2}$  representation of  $\mathfrak{p}$ —an object which has already been well-established in the twistor program of Penrose [145] and in earlier studies such as [146]. To define this representation, we fix our convention for  $\gamma$  matrices in the Weyl basis

$$\gamma^\mu = \begin{bmatrix} \mathbb{0} & \sigma^\mu \\ \bar{\sigma}^\mu & \mathbb{0} \end{bmatrix}, \quad (\text{C.7})$$

where  $\sigma^\mu = (\mathbb{1}, \vec{\sigma})$ ,  $\bar{\sigma}^\mu = (-\mathbb{1}, \vec{\sigma})$ , and  $\vec{\sigma}$  represents the  $2 \times 2$  Pauli matrices

$$\sigma^1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad \sigma^2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \quad \sigma^3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \quad (\text{C.8})$$

The Clifford algebra relation  $\{\gamma^\mu, \gamma^\nu\} = 2\eta^{\mu\nu}\mathbb{1}_{4 \times 4}$  is thus satisfied for  $\eta^{\mu\nu}$  of signature  $(-+++)$ . Chiral projection operators  $\chi_s$  for  $s \in \{L, R\}$  are defined by

$$\chi_L = \frac{1}{2}(\mathbb{1} - \gamma^5) \quad \text{and} \quad \chi_R = \frac{1}{2}(\mathbb{1} + \gamma^5), \quad (\text{C.9})$$

where  $\gamma^5 = i\gamma^0\gamma^1\gamma^2\gamma^3$ . For convenience, we recall several properties of the  $\gamma$  and  $\chi$  matrices:

$$\begin{aligned} \text{(i)} \quad & (\gamma^\mu)^\dagger = \gamma^0\gamma^\mu\gamma^0, \quad \{\gamma^\mu, \gamma^5\} = \mathbb{0} \quad \text{and} \quad (\gamma^5)^2 = \mathbb{1} \\ \text{(ii)} \quad & \chi_R\gamma^\mu = \gamma^\mu\chi_L \quad \text{and} \quad \chi_L\gamma^\mu = \gamma^\mu\chi_R \\ \text{(iii)} \quad & \chi_s^\dagger = \chi_s = \chi_s^2, \quad \chi_R + \chi_L = \mathbb{1}, \quad \text{and} \quad \chi_R\chi_L = \chi_L\chi_R = \mathbb{0}, \end{aligned} \quad (\text{C.10})$$

where  $\dagger$  denotes a conjugate transpose.

The *twistor representation*  $\rho_s^T : \mathfrak{p} \rightarrow \mathfrak{gl}_4(\mathbb{C})$  may now be defined as follows:

$$\begin{aligned} P^\alpha &:= \gamma^\alpha\chi_s \\ M^{\alpha\beta} &:= \frac{1}{4}[\gamma^\alpha, \gamma^\beta]. \end{aligned} \quad (\text{C.11})$$

Eq. (C.11) defines two distinct chiral representations of the Poincaré Lie algebra—distinguished by  $s \in \{L, R\}$ —both satisfying the Lie bracket of Eq. (C.2). Matrices of these representations are of the general form

$$\begin{bmatrix} Z & \mathbb{0} \\ X & -Z^\dagger \end{bmatrix} \in \rho_L^T(\mathfrak{p}) \quad \text{and} \quad \begin{bmatrix} Z & X \\ \mathbb{0} & -Z^\dagger \end{bmatrix} \in \rho_R^T(\mathfrak{p}), \quad (\text{C.12})$$

where  $Z \in \mathfrak{sl}_2(\mathbb{C})$  is traceless and comprises six Lorentz degrees of freedom (DOF) while  $X = X^\dagger$  is Hermitian and comprises four translation DOF. It can be shown  $\forall A \in \rho_s^T(\mathfrak{p})$  and  $g \in \rho_s^T(\mathbb{P})$  that

$$\begin{aligned} A^\dagger \gamma^0 + \gamma^0 A &= 0 \\ g^\dagger \gamma^0 g &= \gamma^0. \end{aligned} \tag{C.13}$$

We observe that, due to our choice of convention in Eq. (C.7),  $\gamma^0$  is the matrix of a canonical symplectic form,  $\gamma^0 = [\mathbb{0} \ \mathbb{1}; -\mathbb{1} \ \mathbb{0}]$ .

In  $\mathbb{1}$ -loop theory, the Poincaré symmetries of spacetime are reinterpreted as internal gauge symmetries of matter fields. In particular, rather than view Eq. (C.11) as defining generators of Poincaré symmetries on a complex spacetime, we regard it as the representation of a spin- $\frac{1}{2}$  matter field. We thus proceed with the algebraic—rather than geometric—aspects of the twistor program in mind.

We denote the twistor matter field as  $\psi[\mathbf{n}]$  and define its Poincaré transformation  $\forall g[\mathbf{n}] \in \rho_s^T(\mathbb{P})$  as follows:

$$\begin{aligned} \psi'[\mathbf{n}] &= g[\mathbf{n}] \triangleright \psi[\mathbf{n}] \\ &= \exp(\Gamma, e)[\mathbf{n}] \triangleright \psi[\mathbf{n}] \\ &= \exp\left(\frac{1}{2}\Gamma_{\mu\nu}[\mathbf{n}]M^{\mu\nu} + e_\mu[\mathbf{n}]P^\mu\right) \psi[\mathbf{n}] \\ &= \exp\left(\frac{1}{4}\Gamma_{\mu\nu}\gamma^{\mu\nu} + \not{e}\chi_s\right) \psi \end{aligned} \tag{C.14}$$

where  $\gamma^{\mu\nu} = \frac{1}{2}[\gamma^\mu, \gamma^\nu]$ ,  $\not{e} = e_\mu[\mathbf{n}]\gamma^\mu$  in Feynman notation, and  $s \in \{L, R\}$  is determined by the chirality of our representation—that is, by the chirality of  $\psi$ .

At this point, our development looks entirely analogous to 5-vector theory: We have defined a finite-dimensional matter field representation of  $\mathfrak{p}$ . However, we now endeavor to form a  $\rho_s^T(\mathfrak{p})$ -valued current  $\mathcal{J}$ , and in so doing find that  $U(2, 2) \supset \mathbb{P}$  is a more natural gauge group for a  $\mathbb{1}$ -loop theory of twistors.

### C.3.2 The 1-loop current

We attempt to construct a  $\rho_s^T(\mathfrak{p})$ -valued 1-loop current from the twistor field. As above,  $\mathcal{J}_a$  must be a function of neighboring matter fields— $\mathcal{J}_a[\mathbf{n}] = \mathcal{J}(\psi, \psi_a^+)$  where  $\psi_a^+[\mathbf{n}] = U_a^{-1}[\mathbf{n}]\psi[\mathbf{n} + \hat{a}]$ —and valued in the adjoint representation corresponding to  $\rho_s^T(\mathfrak{p})$ . To satisfy these requirements,  $\mathcal{J}_a[\mathbf{n}]$  can be defined as follows:

$$\mathcal{J}_a[\mathbf{n}] = \frac{i}{2} \left( \psi \bar{\psi}_a^+ - \psi_a^+ \bar{\psi} \right) \quad (\text{C.15})$$

where  $\bar{\psi}[\mathbf{n}] = \psi^\dagger[\mathbf{n}]\gamma^0$ . Given Eq. (C.13),  $\mathcal{J}_a$  clearly transforms adjointly; indeed, for any  $\Psi_g$  with  $g \in \rho_s^T(\mathbb{P})$ , the relation  $\text{Ad}_g \circ \mathcal{J} = \mathcal{J} \circ \Psi_g$  holds. (In fact, any bilinear  $\psi_1 \bar{\psi}_2$  satisfies this requirement, much like  $\Phi_1 \Phi_2^T \eta_0$  in Eq. (C.5).) We further note that when  $\psi_a^+[\mathbf{n}] = \alpha \psi[\mathbf{n}]$ , we have  $\mathcal{J}_a[\mathbf{n}] = 0 \ \forall \alpha \in \mathbb{R}$ . A similar result obtains for the 5-vector in Eq. (C.5), whose  $\rho_5(\mathfrak{p})$ -valued current vanishes whenever  $\Phi_a^+[\mathbf{n}] \propto \Phi[\mathbf{n}]$ .

However, Eq. (C.15) is not necessarily  $\rho_s^T(\mathfrak{p})$ -valued just yet. In particular,  $\psi$  and  $\psi_a^+$  comprise 16 real DOF altogether. To establish a  $\rho_s^T(\mathfrak{p})$ -valued current with ten DOF, six constraints must be satisfied. Using 2-spinors  $\xi_s$  and  $\lambda_s$  to denote  $\psi = \begin{bmatrix} \xi_L \\ \xi_R \end{bmatrix}$  and  $\psi_a^+ = \begin{bmatrix} \lambda_L \\ \lambda_R \end{bmatrix}$ , we can ensure that  $\mathcal{J}_a$  conforms with Eq. (C.12) by imposing the following additional constraints:

$$\begin{aligned} \xi_{\bar{s}} \lambda_s^\dagger - \lambda_{\bar{s}} \xi_s^\dagger &= 0 & (4 \text{ constraints}) \\ \xi_s^\dagger \lambda_{\bar{s}} - \lambda_s^\dagger \xi_{\bar{s}} &= 0 & (2 \text{ constraints}) \end{aligned} \quad (\text{C.16})$$

where  $\bar{s}$  toggles  $s$ . Together, Eqs. (C.15)-(C.16) now define a  $\rho_s^T(\mathfrak{p})$ -valued 1-loop current. For example, fixing  $s = L$ ,

$$\mathcal{J}_a[\mathbf{n}] = \frac{i}{2} \left[ \begin{array}{c|c} \lambda_L \xi_R^\dagger - \xi_L \lambda_R^\dagger & 0 \\ \hline \lambda_R \xi_R^\dagger - \xi_R \lambda_R^\dagger & \xi_R \lambda_L^\dagger - \lambda_R \xi_L^\dagger \end{array} \right] \quad (\text{C.17})$$

as desired, where the constraints of Eq. (C.16) enforce the vanishing of the top right quadrant  $\mathcal{J}_a^{12}[\mathbf{n}] = 0$ , and  $\mathbf{Tr}[\mathcal{J}_a^{11}] = \mathbf{Tr}[\mathcal{J}_a^{22}] = 0$ .

The necessity of these contrived constraints suggests that the Poincaré group is not a natural gauge group for a twistor  $\mathbb{1}$ -loop theory. No unconstrained linear combination of  $\psi\bar{\psi}_a^+$  and  $\psi_a^+\bar{\psi}$  yields a current  $\mathcal{J}_a$  with sufficient freedom to describe a ten-parameter Poincaré current, without overshooting to introduce all 16 DOF of this pair of twistors. Although  $\rho_s^T(\mathbf{p})$  readily forms a Poincaré representation, therefore, its misfit as a  $\mathbb{1}$ -loop current invites us to view this representation as part of a larger group structure. Thus, it bears investigating the consequences of relaxing the constraints above.

## C.4 From $\mathbb{P}$ to $U(2, 2)$ : Unconstraining the $\mathbb{1}$ -Loop Current

Before we entirely abandon the constraints of Eq. (C.16), let us consider how electromagnetism might be incorporated into a twistor  $\mathbb{1}$ -loop theory. We straightforwardly embellish our definition of the twistor representation to include  $U(1)$  gauge transformations as follows:

$$\begin{aligned}\psi'[\mathbf{n}] &= g[\mathbf{n}] \triangleright \psi[\mathbf{n}] \\ &= \exp(\Gamma, e, \theta)[\mathbf{n}] \triangleright \psi[\mathbf{n}] \\ &= e^{i\theta} \exp\left(\frac{1}{4}\Gamma_{\mu\nu}\gamma^{\mu\nu} + \phi\chi_s\right)\psi.\end{aligned}\tag{C.18}$$

The action of  $e^{i\theta}$  in Eq. (C.18) requires the extension of the  $\rho_s^T(\mathbf{p})$  twistor representation to  $\rho_s^T(\mathbf{p} \oplus \mathbf{u}(1))$ . This can be achieved by including with Eq. (C.11) the following

$4 \times 4$  matrix generator of  $U(1)$  transformations:

$$R := i\mathbb{1}. \quad (\text{C.19})$$

With  $R$ , the submatrix  $Z$  in Eq. (C.12) can acquire a nonvanishing imaginary trace. To generalize  $\mathcal{J}_a$  accordingly, we may leave its definition in Eq. (C.15) unchanged and simply relax the latter constraint of Eq. (C.16) to

$$\mathbf{Im} [\xi_s^\dagger \lambda_{\bar{s}} - \lambda_s^\dagger \xi_{\bar{s}}] = 0 \quad (1 \text{ constraint}). \quad (\text{C.20})$$

Recalling the factor of  $i$  in Eq. (C.15), this relaxation affords an imaginary diagonal in  $\mathcal{J}_a$ , i.e.,  $\mathbf{diag}[\mathcal{J}_a] = \frac{i}{4}\alpha_a\mathbb{1}$  for  $\alpha_a \in \mathbb{R}$ :

$$\mathbf{Tr}[\mathcal{J}_a] = i\alpha_a = \frac{i}{2} (\bar{\psi}_a^+ \psi - \bar{\psi} \psi_a^+). \quad (\text{C.21})$$

As such,  $\mathcal{J}_a$  is now an 11-parameter current. We observe that Eqs. (C.15)-(C.16) are invariant under the  $U(1)$  transformation of Eq. (C.18). Therefore, since the abelian adjoint action of  $U(1)$  is trivial,  $\mathcal{J}_a$  as defined in Eq. (C.15) continues to satisfy  $\mathbf{Ad}_g \circ \mathcal{J} = \mathcal{J} \circ \Psi_g$  for all  $g \in \rho_s^T(\mathbb{P} \times U(1))$ .

It is worth noting that Eq. (C.21) roughly resembles the electromagnetic current of a chiral fermion in continuous spacetime. In particular, if we let  $\psi[\mathbf{n} + \hat{a}] \approx \psi[\mathbf{n}]$  and set  $U_a[\mathbf{n}] = \exp(eA_a[\mathbf{n}])$  on a rectified neighborhood [49]—such that  $A_a[\mathbf{n}] = (\Gamma_{\nu a}^\mu[\mathbf{n}], e_{\mu a}[\mathbf{n}], \theta_a[\mathbf{n}]) = (0, \eta_{\mu a}, 0)$  in the notation of Eq. (C.18)—we find:

$$\begin{aligned} \alpha_a &\approx \frac{1}{2} \left[ (U_a^{-1}\psi)^\dagger \gamma^0 \psi - \psi^\dagger \gamma^0 U_a^{-1}\psi \right] \\ &= \frac{1}{2} \left[ \psi^\dagger (\mathbb{1} - ee_{\mu a} \gamma^\mu \chi_s)^\dagger \gamma^0 \psi - \psi^\dagger \gamma^0 (\mathbb{1} - ee_{\mu a} \gamma^\mu \chi_s) \psi \right] \\ &= e\bar{\psi}_s \gamma_a \psi_s, \end{aligned} \quad (\text{C.22})$$

where we have applied the identities of Eq. (C.10) and denoted  $\gamma_a = \gamma^\mu \eta_{\mu a}$  and  $\psi_s = \chi_s \psi$ . This is a first hint that physics analogous to QED might appear in a twistor 1-loop theory with  $\mathcal{J}_a$  appropriately unconstrained.

Pursuing this course to its natural conclusion, we now explore the Lie algebra that arises when all six constraints of Eq. (C.16) are relaxed. In this circumstance, the value of  $\mathcal{J}_a$  in Eq. (C.15) is spanned by the following 16-dimensional basis of generators:

$$\begin{aligned}
P^\alpha &:= \gamma^\alpha \chi_s & D &:= \frac{s^\pm}{2} \gamma^5 \\
K^\alpha &:= \gamma^\alpha \chi_{\bar{s}} & R &:= i\mathbb{1}. \\
M^{\alpha\beta} &:= \frac{1}{4} [\gamma^\alpha, \gamma^\beta]
\end{aligned} \tag{C.23}$$

where  $s^\pm = \delta_{sL} - \delta_{sR}$ . These satisfy the following Lie algebra:

$$\begin{aligned}
[P^\alpha, P^\beta] &= 0 \\
[K^\alpha, K^\beta] &= 0 \\
[M^{\alpha\beta}, M^{\mu\nu}] &= \eta^{\beta\mu} M^{\alpha\nu} + \eta^{\alpha\nu} M^{\beta\mu} - \eta^{\alpha\mu} M^{\beta\nu} - \eta^{\beta\nu} M^{\alpha\mu} \\
[M^{\alpha\beta}, P^\mu] &= \eta^{\beta\mu} P^\alpha - \eta^{\alpha\mu} P^\beta \\
[M^{\alpha\beta}, K^\mu] &= \eta^{\beta\mu} K^\alpha - \eta^{\alpha\mu} K^\beta \\
[P^\alpha, K^\beta] &= 2(M^{\alpha\beta} + \eta^{\alpha\beta} D) \\
[D, P^\alpha] &= P^\alpha \\
[D, K^\alpha] &= -K^\alpha \\
[D, M^{\alpha\beta}] &= 0 \\
[R, \cdot] &= 0.
\end{aligned} \tag{C.24}$$

When exponentiated, the generators of Eq. (C.23) form the connected group of conjugate symplectic matrices  $Sp^*(4, \mathbb{C})$ , constituted by all matrices satisfying

Eq. (C.13), that is  $Sp^*(4, \mathbb{C}) = \{g \mid g^\dagger \gamma^0 g = \gamma^0\}$ . In this sense, they fully exploit the symmetries of the twistor representation in  $\mathbb{1}$ -loop theory. We note that  $Sp^*(4, \mathbb{C}) \cong U(2, 2)$ , where the latter denotes the group of pseudo-unitary matrices  $U(2, 2) = \{h \mid h^\dagger \eta_{2,2} h = \eta_{2,2}\}$  for  $\eta_{2,2} = \mathbf{diag}(1, 1, -1, -1)$ . The isomorphism between these groups may be given by [147]

$$g = UhU^\dagger \quad \text{where} \quad U = \frac{1}{\sqrt{2}} \begin{bmatrix} \mathbb{1} & \mathbb{1} \\ i\mathbb{1} & -i\mathbb{1} \end{bmatrix} \quad (\text{C.25})$$

is unitary and  $U^\dagger \gamma^0 U = i\eta_{2,2}$ . Despite our preference for  $\mathfrak{sp}^*(4, \mathbb{C})$  in matrix calculations, we defer to the name  $\mathfrak{u}(2, 2) = \mathfrak{su}(2, 2) \oplus \mathfrak{u}(1)$  to emphasize that it contains the conformal Lie algebra. We denote this representation  $\rho_s^T : \mathfrak{u}(2, 2) \rightarrow \mathfrak{gl}_4(\mathbb{C})$  so that  $\mathcal{J}_a$  is a  $\rho_s^T(\mathfrak{u}(2, 2))$ -valued current. The conformal group  $SU(2, 2)$  is simple and constitutes the smallest semi-simple group containing the Poincaré group [148].

When regarded as transformations of a Minkowski spacetime,  $K^\alpha$  are geometrically interpreted as special conformal transformations (SCTs). In the context of  $\mathbb{1}$ -loop theory, however,  $K^\alpha$  arises algebraically as though a mere translation with chirality opposite that of  $P^\alpha$ .  $D$  is a generator of dilations, and the central element  $R$  is a generator of  $U(1)$  transformations. An arbitrary matrix element of  $\rho_s^T(\mathfrak{u}(2, 2))$  is of the form

$$\begin{bmatrix} Z & X \\ Y & -Z^\dagger \end{bmatrix} \in \rho_s^T(\mathfrak{u}(2, 2)) \quad (\text{C.26})$$

for  $X = X^\dagger$  and  $Y = Y^\dagger$  Hermitian (4 DOF each) and  $Z \in \mathfrak{gl}_2(\mathbb{C})$  arbitrary (8 DOF). If we fix  $s = R$  such that  $P^\mu = \gamma^\mu \chi_R$  and  $K^\mu = \gamma^\mu \chi_L$ , then  $X, Y$  and  $Z$  above comprise the DOF of  $\{P^\mu\}$ ,  $\{K^\mu\}$ , and  $\{M^{\mu\nu}, D, R\}$ , respectively.

## C.5 Interactions in $U(2, 2)$ 1-Loop Theory

Let us more closely examine a generic  $\mathfrak{u}(2, 2)$  current,

$$\mathcal{J}(\psi_1, \psi_2) = \frac{i}{2}(\psi_1 \bar{\psi}_2 - \psi_2 \bar{\psi}_1). \quad (\text{C.27})$$

It is clear that the image of  $\mathcal{J}$  is a proper subset of the Lie algebra, in particular,

$$\text{Im}[\mathcal{J}] = \{A \in \rho_s^T(\mathfrak{u}(2, 2)) \mid \mathbf{rank}[A] \leq 2\}. \quad (\text{C.28})$$

This fact has interesting consequences for the set of permissible interactions in twistor 1-loop theory.

As a particularly illustrative example, suppose we attempt to model an electromagnetic interaction in our theory by defining a nontrivial  $U(1)$  curvature at some vertex  $\mathbf{n}$ . Examining the  $U(1)$  generator  $R$ , we note that  $\mathbf{rank}[R] = 4$ . Thus, no solution  $J_a[\mathbf{n}] = \exp(\mathcal{J}_a[\mathbf{n}])$  can be found for the 1-loop equation  $\delta\Omega_a[\mathbf{n}] \cdot J_a[\mathbf{n}] = \mathbb{1}$  when  $\delta\Omega_a[\mathbf{n}] = \exp[\epsilon R]$  for  $\epsilon \in \mathbb{R}$ . Simply put, in 1-loop theory the twistor field cannot couple to  $U(1)$  curvature alone. On the other hand, we find that  $R + 2M^{ij} \in \text{Im}[\mathcal{J}] \forall 1 \leq i \neq j \leq 3$ , since  $\mathbf{rank}[R + 2M^{ij}] = 2$ . Thus, the twistor field *can* couple to  $\delta\Omega_a[\mathbf{n}]$  when it is valued in the one-parameter subgroup  $\exp[\epsilon(R + 2M^{ij})]$  and its adjoint orbit in  $\rho_s^T(U(2, 2))$ .

To better understand the dynamics of the matter field in such an interaction, we first solve  $\mathcal{J}$  for  $\psi_2$ . In particular, we suppose  $\psi_1 \in \mathbb{C}^4$  and  $\mathcal{J}_0 \in \rho_s^T(\mathfrak{u}(2, 2))$  are known quantities, and that  $\psi_1$  satisfies the gauge-invariant normalization  $\bar{\psi}_1 \psi_1 = 2im$  for  $m \neq 0$ . (Since  $(\bar{\psi}\psi)^\dagger = -\bar{\psi}\psi$ , it follows that  $m \in \mathbb{R}$ .) Assuming  $\mathcal{J}_0 \in \text{Im}[\mathcal{J}]$ , we solve for  $\psi_2$  such that  $\mathcal{J}(\psi_1, \psi_2) = \mathcal{J}_0$ .

Setting  $\mathcal{J}_0 = \frac{i}{2}(\psi_1\bar{\psi}_2 - \psi_2\bar{\psi}_1)$ , we first note that

$$\Pi_1 [\mathcal{J}_0\psi_1] = m\Pi_1\psi_2 \quad (\text{C.29})$$

where  $\Pi_1$  denotes the projection with kernel  $\psi_1$ ,

$$\Pi_1 = \mathbb{1} - \frac{1}{2im}\psi_1\bar{\psi}_1. \quad (\text{C.30})$$

This specifies  $\psi_2$  in three complex dimensions, but leaves its contribution from  $i\psi_1$  unspecified. Solving for this contribution, we find:

$$\psi_2 = \left[ \left( \beta + \frac{i}{4m^2}\bar{\psi}_1\mathcal{J}_0\psi_1 \right) \mathbb{1} + \frac{1}{m}\mathcal{J}_0 \right] \psi_1 \quad (\text{C.31})$$

for  $\beta \in \mathbb{R}$  arbitrary. (Adding any real multiple of  $\psi_1$  to  $\psi_2$  leaves  $\mathcal{J}$  invariant.) If we now require that  $\bar{\psi}_2\psi_2 = 2im$  and recall that  $\gamma^0\mathcal{J}_0^\dagger\gamma^0 = \mathcal{J}_0$  as in Eq. (C.13), we have

$$\beta = \sqrt{1 - \frac{i}{2m^3}\bar{\psi}_1\mathcal{J}_0^2\psi_1 + \frac{3}{16m^4}(\bar{\psi}_1\mathcal{J}_0\psi_1)^2} \quad (\text{C.32})$$

where  $\mathbf{sign}(\beta)$  is determined by requiring that  $\psi_2 = \psi_1$  when  $\mathcal{J}_0 = \mathbb{0}$ . Eqs. (C.31)-(C.32) solve  $\mathcal{J}(\psi_1, \psi_2) = \mathcal{J}_0$  for  $\psi_2$ , assuming  $\mathcal{J}_0 \in \text{Im}[\mathcal{J}]$ .

# Appendix D

## Discretization of the Tetradic Palatini Action

### D.1 Introduction

In this appendix, we develop a new structure-preserving algorithm for the general relativistic simulation of gravitational systems in vacuum. We work in a Lagrangian formalism to derive a variational algorithm from a novel discretization of the tetradic Palatini action [149].

Structure-preserving discretizations of general relativity (GR) have a long history. The most widely explored such technique was introduced in 1961: Regge calculus [150] is a discrete variational approximation of GR that encodes spacetime data on a simplicial mesh. In four spacetime dimensions, Regge calculus elegantly approximates the Einstein-Hilbert action by a sum over areas  $A_h$  and *deficit angles*  $\delta_h$ , such that

$$S_{\text{Regge}} = \sum_h A_h \delta_h \xrightarrow{A_h \rightarrow 0} S_{\text{EH}} = \frac{1}{2} \int d^4x \sqrt{-g} R \quad (\text{D.1})$$

in the continuum limit. Here,  $h$  labels each 2-simplex (i.e. triangle) of the simplicial complex, and  $\delta_h$  describes the failure of the 4-simplices adjoining  $h$ —i.e.

$\{\sigma^4 \mid \sigma^4 \supset h\}$ —to tessellate their embedding in flat  $\mathbb{R}^4$  spacetime [151].

Since the 1970s, Regge calculus has not only been actively employed as the basis of many studies in quantum gravity (e.g. [152–157]) but also as an algorithmic approach to classical numerical relativity (e.g. [158–166]). Despite its many successes as a numerical tool, however, most studies in numerical relativity continue to depend on standard finite difference methods. Two reasons cited for this include the need to develop (i) a description of matter in Regge calculus, as well as (ii) a better understanding of its relationship to standard methods in numerical relativity [167, 168].

In particular, because the degrees of freedom of Regge calculus are quite distinct from those of continuum GR, it can be challenging to initialize a Regge calculus simulation with known GR initial conditions, or to test whether a particular simulation using Regge calculus recovers a known GR solution. Although various physical solutions have indeed been thoroughly and successfully benchmarked with Regge calculus [169, 170], it would seem that any given simulation generally requires a bespoke understanding of the map between discrete and continuum degrees of freedom.

It is also worth noting that, despite Regge calculus being a variational method, it nonetheless forfeits—in its complete, nonperturbative formulation—the local gauge symmetry of GR [155]. While local gauge symmetry is maintained in a Regge calculus description of flat spacetime—and even in a linearized Regge calculus of curved spacetimes [171]—this structural feature of GR is at best only partially preserved overall.

In this paper, an alternative variational approach to simulating general relativity is developed that ameliorates some of these limitations. Our effort employs familiar tools of lattice gauge theory [133] to construct a structure-preserving discretization of the tetradic Palatini action [149]. Using a Poincaré group valued connection, we describe a variational algorithm that exactly preserves Lorentz gauge symmetry, and

we characterize its symplectic structure.

The approach we take is very closely related to Poincaré gauge theoretic studies of lattice quantum gravity by Menotti, et al. [140, 172]. To our knowledge, however, the classical physics of these methods, including their equations of motion, for example, have not previously been explored, nor have they been extended to define an algorithm for numerical relativity. Moreover, our construction is general to simplicial and hypercubic discretizations of spacetime, and we develop a somewhat streamlined construction of the aforementioned Poincaré connection.

## D.2 The Tetradic Palatini Action in Continuous Spacetime

We begin our discussion in continuous spacetime using the following index conventions:

- internal Lorentz indices are denoted  $\{A, B, \dots\}$ , raised and lowered by the Minkowski metric  $\eta_{AB}$ ;
- spacetime indices are denoted  $\{\mu, \nu, \dots\}$ , raised and lowered by the metric  $g_{\mu\nu} = \eta_{AB} e_\mu^A e_\nu^B$ ; and
- any other indices  $\{a, b, \dots\}$  will be specified as needed.

On a four-dimensional spacetime  $M$ , the tetrad (or vierbein) may be defined as a vector valued 1-form with components  $e^A \in \Gamma(\wedge^1 T^*M)$  such that  $e_\mu^A(x)$  defines an isomorphism between the tangent space  $T_x M$  and the internal Lorentz space at  $x \forall x \in M$ . The vierbein in turn determines a metric on  $M$  according to the relation

$$g_{\mu\nu} = e_\mu^A \eta_{AB} e_\nu^B. \tag{D.2}$$

We further introduce the  $\mathfrak{so}(3, 1)$ -valued 1-form with components  $\omega_B^A \in \Gamma(\wedge^1 T^* M)$ , also called the spin connection. Its curvature  $F_B^A \in \Gamma(\wedge^2 T^* M)$  is defined by

$$F_B^A = D\omega_B^A = d\omega_B^A + \frac{1}{2}[\omega, \omega]_B^A \quad (\text{D.3})$$

where  $[\cdot, \cdot]$  extends the conventional Lie bracket to Lie algebra-valued differential forms via coefficient multiplication [43].

The Lagrangian  $\mathcal{L} \in \Gamma(\wedge^4 T^* M)$  of the tetradic Palatini action  $\mathcal{S} = \int_M \mathcal{L}$  is now defined in terms of the vierbein and spin connection by [149]

$$\mathcal{L} = \epsilon_{ABCD} (e^A \wedge e^B \wedge F^{CD}). \quad (\text{D.4})$$

The Lorentz invariance of  $\mathcal{L}$  immediately follows from the  $SO(3, 1)$  invariance of the Levi-Civita symbol  $\epsilon_{ABCD}$ .

Unlike the metric and connection  $(g, \Gamma)$  of the Einstein-Hilbert action, the fields  $(e, \omega)$  of Eq. (D.4) are taken to be independent and varied accordingly. Variation of each field yields the respective equations of motion

$$\begin{aligned} (\delta e) : \quad 0 &= \epsilon_{ABCD} e^B \wedge F^{CD} \\ (\delta \omega) : \quad 0 &= \epsilon_{ABCD} (De^A \wedge e^B - e^A \wedge De^B), \end{aligned} \quad (\text{D.5})$$

where

$$De^A = de^A + \omega_B^A \wedge e^B. \quad (\text{D.6})$$

The former relation of Eq. (D.5) yields Einstein's vacuum field equations while the latter is equivalent to a zero torsion condition. Despite having fewer initial assumptions (such as zero torsion), the tetradic Palatini action nevertheless recovers the equations of motion of GR in vacuum.

The following observation will also be useful in the next section that discretizes  $\mathcal{L}$ . Evaluated on a 4-tuple of vector fields— $\mathbf{X} = (X_1, X_2, X_3, X_4)$ ,  $X_a \in \Gamma(TM)$ —the 4-form  $\mathcal{L}$  of Eq. (D.4) gives

$$\begin{aligned}\mathcal{L}(\mathbf{X}) &= \frac{1}{2} \epsilon_{ABCD} (e_\mu^A e_\nu^B F_{\sigma\tau}^{CD}) \epsilon^{abcd} X_a^\mu X_b^\nu X_c^\sigma X_d^\tau \\ &= \frac{1}{2} \epsilon_{ABCD} (e_\mu^A e_\nu^B F_{\sigma\tau}^{CD}) \epsilon^{\mu\nu\sigma\tau} \det \mathbf{X}\end{aligned}\tag{D.7}$$

where the function  $\det \mathbf{X}$  is the matrix determinant of the 4-tuple, evaluated pointwise over  $M$ .

### D.3 The Discrete Action

We now reformulate the Lagrangian of the previous section in a discrete setting. Our formalism is general to orientable simplicial and cubic discretizations. We denote the set of all  $k$ -cells  $\Sigma^k = \{\sigma^k\}$ , such that any oriented  $k$ -cell will be denoted  $\sigma^k$  or will otherwise be specified by an ordered label of its vertices.  $\sigma_{ij} \in \Sigma^1$ , for example, denotes an edge oriented from vertex  $\sigma_i \in \Sigma^0$  to vertex  $\sigma_j \in \Sigma^0$ . We define  $N_i(\sigma^k) = \{j \neq i \mid \sigma_{ij} \subset \sigma^k\}$  as the set of labels of neighboring vertices in the cell  $\sigma^k$  that share an edge with basepoint  $\sigma_i$ . In both simplicial and cubic discretizations in four dimensions, for example,  $\#N_i(\sigma^4) = 4$  if  $\sigma_i \subset \sigma^4$  and 0 otherwise. We denote the permutation set of these neighboring vertex labels as  $\Pi_i(\sigma^4) = S[N_i(\sigma^4)]$ .

We now define a Poincaré group-valued connection  $U(\sigma_{ij}) = U_{ij}$  along each edge  $\sigma^1 \in \Sigma^1$ . Its representation  $SO(3, 1) \times \mathbb{R}^4 \rightarrow GL_5(\mathbb{R})$  is defined such that the Poincaré group element  $(\Lambda, \ell)$  characterizing the Lorentz transformation  $\Lambda$  and the translation  $\ell$  yields the following connection:

$$U_{ij} = \begin{bmatrix} \Lambda_{ij} & \ell_{ij} \\ \mathbf{0} & 1 \end{bmatrix} \quad \text{s.t.} \quad U_{ji} = U_{ij}^{-1} = \begin{bmatrix} \Lambda_{ij}^{-1} & -\Lambda_{ij}^{-1} \ell_{ij} \\ \mathbf{0} & 1 \end{bmatrix}.\tag{D.8}$$

The edge data  $\Lambda_{ij} \in SO(3, 1)$  and  $\ell_{ij} \in \mathbb{R}^4$  will comprise the degrees of freedom of our discrete action. We note that  $\Lambda_{ji} = (\Lambda_{ij})^{-1}$  and  $\ell_{ji} = -\Lambda_{ji}\ell_{ij}$  above.

For notational ease, we define the connection along each edge  $U(\sigma^1)$  to act from the right. Therefore, given an arbitrary Lorentz gauge transformation defined at each vertex, say

$$\{g_i = g(\sigma_i) \in SO(3, 1) \forall \sigma_i \in \Sigma^0\}, \quad (\text{D.9})$$

the connection  $U_{ij}$  transforms as

$$\begin{aligned} U'_{ij} &= \begin{bmatrix} g_i & \mathbf{0} \\ \mathbf{0} & 1 \end{bmatrix}^{-1} U_{ij} \begin{bmatrix} g_j & \mathbf{0} \\ \mathbf{0} & 1 \end{bmatrix} \\ &= \left[ \begin{array}{c|c} g_i^{-1}\Lambda_{ij}g_j & g_i^{-1}\ell_{ij} \\ \hline \mathbf{0} & 1 \end{array} \right]. \end{aligned} \quad (\text{D.10})$$

We denote the  $(A, B)^{\text{th}}$  component of the Lorentz connection along edge  $\sigma_{ij}$  by  $\Lambda_{ijB}^A$ , and the  $A^{\text{th}}$  component of the corresponding translation connection by  $\ell_{ij}^A$ . We also adopt a notation for a Lorentz holonomy with an arbitrary number of edges. In particular, for the holonomy comprised of  $(n - 1)$  connections between the vertices  $\sigma_{i_1}, \dots, \sigma_{i_n}$ , we write

$$\begin{aligned} \Lambda_{i_1 \dots i_n B}^A &= \left( \Lambda_{i_1 i_2} \Lambda_{i_2 i_3} \cdots \Lambda_{i_{n-1} i_n} \right)_B^A \\ &= \Lambda_{i_1 i_2 C}^A \Lambda_{i_2 i_3 D}^C \cdots \Lambda_{i_{n-1} i_n B}^E \end{aligned} \quad (\text{D.11})$$

where intermediate Lorentz indices  $\{C, D, \dots, E\}$  are all contracted. When a holonomy is comprised of the connections along the edges of a single face  $\sigma^2 \in \Sigma^2$  (i.e. when it is a “minimal” nontrivial loop), we will use the symbol  $\Omega$  for its Lorentz holonomy rather than  $\Lambda$ , and we will suppress some of its indices. In particular, given a loop

$\sigma_i \sigma_j \cdots \sigma_k \sigma_i$  around a single face, we denote its holonomy  $\Omega_{ijkB}^A$ . This notation is general to the simplicial and cubic setting, such that, for example,

$$\begin{aligned} \text{Simplicial: } \Omega_{ijk}^{AB} &= (\Lambda_{ij} \Lambda_{jk} \Lambda_{ki})^A {}_C \eta^{CB} \\ \text{Cubic: } \Omega_{ijk}^{AB} &= (\Lambda_{ij} \Lambda_{j'i'} \Lambda_{i'k} \Lambda_{ki})^A {}_C \eta^{CB}. \end{aligned} \quad (\text{D.12})$$

Here,  $i'$  labels the vertex diagonal to  $i$  on the appropriate face of the cubic lattice; in a more typical notation,  $(i, j, i', k) = (\mathbf{n}, \mathbf{n} + \hat{a}, \mathbf{n} + \hat{a} + \hat{b}, \mathbf{n} + \hat{b})$ .  $\Omega$  thereby characterizes the Lorentz curvature of a face  $\sigma^2$ .

With the preceding notations in mind, we now define the discrete action and Lagrangian on hypercells  $\{\sigma^4\} = \Sigma^4$  as follows:

$$\begin{aligned} S &= \sum_{\sigma^4 \in \Sigma^4} L(\sigma^4) \\ L(\sigma^4) &= \sum_{\substack{\sigma_i \subset \sigma^4 \\ \pi \in \Pi_i(\sigma^4)}} \frac{(-1)^{|\pi|}}{2\rho_f n_v} \epsilon_{ABCD} \left( \ell_{i\pi(1)}^A \ell_{i\pi(2)}^B \Omega_{i\pi(3)\pi(4)}^{CD} \right). \end{aligned} \quad (\text{D.13})$$

The summand of Eq. (D.13) can be roughly understood as evaluating the Lagrangian of Eq. (D.7) on a frame determined by edges adjoining  $\sigma_i$ .  $\pi$  denotes a permutation of these edges whose orientation of parity  $|\pi|$  is inherited from the mesh itself.  $n_v$  denotes the number of vertices per hypercell, so that  $L(\sigma^4)$  averages over frames constructed at each vertex of  $\sigma^4$ .  $\rho_f$  denotes a shape factor that accounts for the hypercell volume in a setting with edges of unit length. The determinant appearing in Eq. (D.7) is now unnecessary; implicit in  $\ell_{ij}^A$  and  $\Omega_{ijk}^{AB}$  are the lengths and areas, respectively, of the discrete connection, providing a volume factor that need only be normalized by  $\rho_f$ . Specifically,  $(\rho_f, n_v) = (12, 5)$  and  $(1, 16)$  in the simplicial and cubic settings, respectively.

Finally, to demonstrate how the group-valued fields of Eq. (D.13) approximate

Eq. (D.7), we note that

$$\begin{bmatrix} \Lambda & \ell \\ \mathbf{0} & 1 \end{bmatrix} = \exp \begin{bmatrix} \omega & e \\ \mathbf{0} & 0 \end{bmatrix} \quad (\text{D.14})$$

for some  $\omega \in \mathfrak{so}(3, 1)$  and  $e \in \mathbb{R}^4$ . Thus,  $\Lambda^A_B \sim \delta^A_B + \omega^A_B$  and  $\ell^A \sim e^A$  to least nontrivial order. Similarly,  $\Omega^{AB} \sim \eta^{AB} + F^{AB}$  for some  $F \in \mathfrak{so}(3, 1)$ , and  $\eta^{AB}$  is annihilated by the Levi-Civita symbol in Eq. (D.13). To leading order, therefore, fields of the discrete Lagrangian recover the Lie algebraic fields of Eq. (D.7).

We further note the local Lorentz invariance of  $L(\sigma^4)$ . In particular, under an arbitrary gauge transformation  $\{g_i \in SO(3, 1)\}_{\sigma_i \in \Sigma^0}$  using Eq. (D.10) we find

$$\begin{aligned} & \left( \epsilon_{ABCD} \ell_{i\pi(1)}^A \ell_{i\pi(2)}^B \Omega_{i\pi(3)\pi(4)}^{CD} \right)' \\ &= \epsilon_{ABCD} (g_i^{-1} \ell_{i\pi(1)})^A (g_i^{-1} \ell_{i\pi(2)})^B (g_i^{-1} \Omega_{i\pi(3)\pi(4)} g_i)^{CD} \\ &= \epsilon_{ABCD} \ell_{i\pi(1)}^A \ell_{i\pi(2)}^B \Omega_{i\pi(3)\pi(4)}^{CD}. \end{aligned} \quad (\text{D.15})$$

The last equality above follows from the Lorentz group relation  $(g_i)^E_F \eta^{FD} = (g_i^{-1})^D_F \eta^{FE}$  and the  $SO(3, 1)$ -invariance of the Levi-Civita symbol.

## D.4 The Discrete Equations of Motion

We now compute equations of motion (EOM) by varying the discrete action with respect to the connection. To compactify notation, when an element of the permutation  $\pi$  appears in an index, it will hereafter be denoted by a corresponding underlined number, for example,  $\underline{1} = \pi(1)$ . As usual in a first-order formalism, we assume  $\Lambda_{ij}$  and  $\ell_{ij}$  to be independent. Varying the action with respect to  $\ell_{ij}^A$ , and applying the

expression for  $U_{ji}$  from Eq. (D.8) where appropriate, we find

$$0 = \frac{\partial S}{\ell_{ij}^A} = \sum_{\sigma^4 \supset \sigma_{ij}} \left[ \sum_{\substack{\pi \in \Pi_i(\sigma^4) \\ \pi(1)=j}} \frac{(-1)^{|\pi|}}{\rho_f n_v} \epsilon_{ABCD} \ell_{i2}^B \Omega_{i34}^{CD} \right. \\ \left. - \sum_{\substack{\pi \in \Pi_j(\sigma^4) \\ \pi(1)=i}} \frac{(-1)^{|\pi|}}{\rho_f n_v} \epsilon_{EBCD} \Lambda_{jiA}^E \ell_{j2}^B \Omega_{j34}^{CD} \right]. \quad (\text{D.16})$$

The first sum of Eq. (D.16) arises from terms with basepoint  $i$  and the second from terms with basepoint  $j$ . We note that although frames are permuted at distinct basepoints in these two lines, their parities are understood to be induced by a global orientation and are therefore mutually consistent. Eq. (D.16) is counterpart to  $(\delta e)$  of Eq. (D.5), and constitutes a discrete reformulation of Einstein's vacuum equations.

We now derive the the Lorentz connection EOM, exercising caution to ensure that the variation of  $\Lambda_{ij}$  is constrained to the  $SO(3,1)$  manifold. In particular,  $\Lambda^T \eta \Lambda = \eta$  implies  $(\Lambda^{-1} \delta \Lambda)^T \eta + \eta (\Lambda^{-1} \delta \Lambda) = 0$ , so that  $\Lambda^{-1} \delta \Lambda \in \mathfrak{so}(3,1)$  for a variation  $\delta \Lambda$ . We can impose this constraint by taking a variation that satisfies  $(\Lambda^{-1} \delta \Lambda)^{AB} = (\Lambda^{-1} \delta \Lambda)^{[AB]}$ , but is otherwise arbitrary.

To that end, we consider as an example the variation of  $\Omega_{i34}^{CD} = (\Lambda_{i3} \Lambda_{34} \Lambda_{4i})^{CD}$  in the simplicial setting with respect to the Lorentz connection on the edge  $\sigma_{i3}$ :

$$\begin{aligned} \delta \Omega_{i34}^{CD} &= (\Lambda_{i3E}^C \Lambda_{3iF}^E) \delta \Lambda_{i3G}^F \Lambda_{34H}^G \Lambda_{4i}^{HD} \\ &= \Lambda_{i3[E]}^C \Lambda_{34i[G]}^D (\Lambda_{3iF}^E \delta \Lambda_{i3}^{FG}) \end{aligned}$$

The term in parentheses on the first line is a conveniently chosen form of the Kronecker delta  $\delta_F^C$ , and the second line follows from the notation of Eq. (D.11) and from asserting the antisymmetry of the variation  $(\Lambda^{-1} \delta \Lambda)^{[EG]}$ . Continuing in this way, noting that  $\Lambda_{ijB}^A = \eta^{AD} \Lambda_{jD}^C \eta_{CB}$ , and denoting  $(-1)^{|\pi|} / \rho_f n_v = a^{|\pi|}$  for brevity, we vary  $S$

with respect to  $(\Lambda_{ji}\delta\Lambda_{ij})^{[MN]}$  to find, in the simplicial case:

$$\begin{aligned}
0 &= \frac{\partial S_{\text{simplicial}}}{(\Lambda_{ji}\delta\Lambda_{ij})^{[MN]}} \\
&= \sum_{\sigma^4 \supset \sigma_{ij}} \left[ \sum_{\substack{\pi \in \Pi_i(\sigma^4) \\ \pi(3)=j}} a^{|\pi|} \epsilon_{ABCD} \ell_{i\bar{1}}^A \ell_{i\bar{2}}^B \left( \Lambda_{i\bar{4}j[M]}\Lambda_{ij|N}^C \right) \right. \\
&+ \sum_{\substack{k \in \sigma^4 \\ k \neq i,j}} \sum_{\substack{\pi \in \Pi_k(\sigma^4) \\ \pi(3)=i \\ \pi(4)=j}} a^{|\pi|} \epsilon_{ABCD} \ell_{k\bar{1}}^A \ell_{k\bar{2}}^B \left( \Lambda_{kj[M]}\Lambda_{kij|N}^C \right) \\
&+ \left. \sum_{\substack{\pi \in \Pi_j(\sigma^4) \\ \pi(4)=i}} a^{|\pi|} \epsilon_{ABC[M]}\ell_{j\bar{1}}^A \ell_{j\bar{2}}^B \left( \Omega_{j\bar{3}i|N}^C \right) \right]. \tag{D.17}
\end{aligned}$$

The first line of Eq. (D.17) arises from terms with basepoint  $i$ , the middle line from terms with basepoint  $k \neq i, j$  in  $\sigma^4$  and the last from terms with basepoint  $j$ . Eq. (D.17) enforces a discrete zero-torsion condition analogous to  $(\delta\omega)$  of Eq. (D.5).

The Lorentz EOM for a cubic discretization follows similarly:

$$\begin{aligned}
0 &= \frac{\partial S_{\text{cubic}}}{(\Lambda_{ji}\delta\Lambda_{ij})^{[MN]}} \\
&= \sum_{\sigma^4 \supset \sigma_{ij}} \left[ \sum_{\substack{\pi \in \Pi_i(\sigma^4) \\ \pi(3)=j}} a^{|\pi|} \epsilon_{ABCD} \ell_{i\bar{1}}^A \ell_{i\bar{2}}^B \left( \Lambda_{i\bar{4}i'j[M]}\Lambda_{ij|N}^C \right) \right. \\
&+ \sum_{\substack{k \in \sigma^4 \\ k \neq i,j}} \sum_{\substack{\pi \in \Pi_k(\sigma^4) \\ \pi(3)=i \\ k'=j}} a^{|\pi|} \epsilon_{ABCD} \ell_{k\bar{1}}^A \ell_{k\bar{2}}^B \left( \Lambda_{k\bar{4}j[M]}\Lambda_{kij|N}^C \right) \\
&+ \sum_{\substack{k \in \sigma^4 \\ k \neq i,j}} \sum_{\substack{\pi \in \Pi_k(\sigma^4) \\ k'=i \\ \pi(4)=j}} a^{|\pi|} \epsilon_{ABCD} \ell_{k\bar{1}}^A \ell_{k\bar{2}}^B \left( \Lambda_{kj[M]}\Lambda_{k\bar{3}ij|N}^C \right) \\
&+ \left. \sum_{\substack{\pi \in \Pi_j(\sigma^4) \\ \pi(4)=i}} \frac{(-1)^{|\pi|}}{\rho_f n_v} \epsilon_{ABC[M]}\ell_{j\bar{1}}^A \ell_{j\bar{2}}^B \left( \Omega_{j\bar{3}i|N}^C \right) \right]. \tag{D.18}
\end{aligned}$$

Eqs. (D.16-D.18) define the desired algorithm for vacuum numerical relativity.

However, while these equations suffice to compute simulation steps in the *bulk*, the evolution of *boundary connections*—including connections along both spacelike and timelike boundaries—still requires some explanation. In particular, even if initial and boundary connections are known a priori, Eqs. (D.16-D.18) involve data from holonomies that generally extend outside of the boundary wall, and are therefore underspecified on the boundary.

The strategy we adopt [173] to derive equations of motion for boundary connections, therefore, is to extend all spacelike and timelike boundary surfaces outward from the bulk, creating a narrow ‘double wall’ of some fiducial thickness  $\epsilon$  around the simulation domain. This double wall is then populated with cells of width  $\epsilon$ , such that connections between an inner wall vertex  $\sigma_{i_{\text{in}}}$  and an outer wall vertex  $\sigma_{i_{\text{out}}}$  will have  $\Lambda_{i_{\text{in}}i_{\text{out}}} \sim \mathbb{1} + \mathcal{O}(\epsilon)$  and  $\ell_{i_{\text{in}}i_{\text{out}}} \sim \mathcal{O}(\epsilon)$ . The connections lying along the outer wall itself are chosen to copy the initial or boundary conditions of the inner wall. Then, equations of motion for the inner wall connections can be derived as usual from Eqs. (D.16-D.18), as they now behave as connections in the bulk. Finally, we take  $\epsilon \rightarrow 0$  in the resulting equations of motion for the (inner wall) boundary connections.

It is worth noting that not all boundary and initial conditions will satisfy the discrete equations of motion. Just as boundary constraints must be satisfied in the continuum theory, care must be taken to ensure that Eqs. (D.16-D.18) are satisfied on the initial surfaces of the discrete theory.

# Conference Presentations of Dissertation Work

1. 2019 Sherwood Fusion Theory Conference: “Toward Plasma Simulations with Exact Conservation of Energy-Momentum and Charge”
2. 2019 61st Annual Meeting of the APS DPP: “The geometric theory of charge conservation in PIC simulations”
3. 2020 PCTS Workshop: Structure-Preserving Geometric Discretization of Physical Systems: “Poincaré Symmetry on a Discrete Lattice”
4. 2020 62nd Annual Meeting of the APS DPP: “One-Loop Theory”
5. 2021 63rd Annual Meeting of the APS DPP: “A New Gauge-Compatible Finite Element PIC Algorithm on an Unstructured Mesh”

# Publications Concomitant with Dissertation Work

1. E. Kur and A.S. Glasser, “Discrete Gravity with Local Lorentz Invariance.” (2022). To be submitted.
2. A.S. Glasser and H. Qin, “A gauge-compatible Hamiltonian splitting algorithm for particle-in-cell simulations using finite element exterior calculus.” arXiv:2110.10346 [physics.plasm-ph] (2021). Submitted for publication.
3. H. Qin, Y. Fu, A.S. Glasser and A. Yahalom, “Spontaneous and explicit parity-time-symmetry breaking in drift wave instabilities.” Phys. Rev. E, 015215 (2021).
4. A.S. Glasser and H. Qin, “One-Loop Theory.” arXiv: 2007.05968 [hep-th] (2020). Submitted for publication.
5. A.S. Glasser and H. Qin, “The geometric theory of charge conservation in particle-in-cell simulations.” J. Plasma Phys. 86, No. 3, 835860303 (2020).
6. A.S. Glasser, A.H. Glasser, R. Conlin and E. Kolemen, “An ideal MHD  $\delta W$  stability analysis that bypasses the Newcomb equation.” Phys. Plasmas 27, 022114 (2020).

7. A.S. Glasser and H. Qin, “Restoring Poincaré Symmetry to the Lattice.” arXiv:1902.04396 [physics.gen-ph] (2019).
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10. S.J. Thomas, M.A. Paluszek, S.A. Cohen and A.S. Glasser, “Nuclear and Future Flight Propulsion—Modeling the Thrust of the Direct Fusion Drive.” AIAA Propulsion and Energy Forum, (2018). Conference paper.
11. A.S. Glasser and E. Kolemen, “A robust solution for the resistive MHD toroidal  $\Delta'$  matrix in near real-time.” *Phys. Plasmas* 25, 082502 (2018).
12. A.S. Glasser, E. Kolemen and A.H. Glasser, “A Riccati solution for the ideal MHD plasma response with applications to real-time stability control.” *Phys. Plasmas* 25, 032507 (2018).

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