Symbolic Detection of Permutation and Parity Symmetries of Evolution Equations

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Moataz Mohamad Alghamdi

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EXAMINATION COMMITTEE PAGE

The thesis of Moataz Mohamad Alghamdi is approved by the examination committee

Committee Chairperson: Professor Diogo Gomes

Committee Members: Professor Shuyu Sun, Professor Raul Tempone

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ABSTRACT

Symbolic Detection of Permutation and Parity Symmetries of Evolution Equations Moataz Alghamdi

We introduce a symbolic computational approach to detecting all permutation and parity symmetries in any general evolution equation, and to generating associated invariant polynomials, from given monomials, under the action of these symmetries. Traditionally, discrete point symmetries of differential equations are systemically found by solving complicated nonlinear systems of partial differential equations; in the presence of Lie symmetries, the process can be simplified further. Here, we show how to find parity- and permutation-type discrete symmetries purely based on algebraic calculations. Furthermore, we show that such symmetries always form groups, thereby allowing for the generation of new group-invariant conserved quantities from known conserved quantities. This work also contains an implementation of the said results in Mathematica. In addition, it includes, as a motivation for this work, an investigation of the connection between variational symmetries, described by local Lie groups, and conserved quantities in Hamiltonian systems.

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LIST OF ABBREVIATIONS

PDE Partial Differential Equation

PDEPV Permutations of Dependent Variables
PINDV Permutations of Independent Variables

PADEP Parity Transformations of Dependent Vari-

ables

PAIND Parity Transformations of Independent Vari-

ables

Chapter 1

Introduction

A turning point in the study of conservation laws of physical systems was the discovery of their intimate connection to symmetries. Previously, conservation laws had been only explored on an ad hoc basis. Emmy Noether, however, was first to propose a systemic procedure for finding conservation laws using symmetries. She showed that any variational symmetry of the Hamiltonian of a Hamiltonian system has a corresponding local conservation law; that is, to explore conservation laws of a Hamiltonian system is to explore the variational symmetries of its Hamiltonian.

This result paved the way for exploiting the well-developed theory of Lie symmetries of differential equations: variational symmetries are best described by local Lie groups. Consequently, there has been a surge in the interest in developing computational packages for this purpose, e.g., DifferentialGeometry (2004), PDEtools, diffdens2009.m, condens2009.m, and GeM (2009) [7] [8]. These packages consist of implementations of algorithms for solving linear determining equations in different computer algebra systems, e.g., Maple and Mathematica. These equations are solved to find the generators of Lie groups, which are then used to construct the Lie group; one then uses another algorithm, based on Noether's theorem, to construct the associated conservation laws.

Noether theorem, however, only works for a small class of PDEs: PDEs admitting a variational principle whose Fréchet derivative is self-adjoint [6]. Hence, developing more general methods for finding conservation laws for other types of PDEs has been of great interest: some work was devoted to improving on Noether's theorem, e.g.,

see Bessel-Hagen (1921) and Boyer (1967); others worked on developing more general results such as the matching and direct methods. Each of these methods works for a particular class of PDEs.

In this thesis, we are interested in developing an algorithm for identifying new conserved quantities through the use of discrete symmetries. We work with general evolution equations of the (standard) form:

$$\partial_t u_1 = f_1(u_i, x_j, \partial_j u_i)$$

$$\partial_t u_2 = f_2(u_i, x_j, \partial_j u_i)$$

$$\partial_t u_3 = f_3(u_i, x_j, \partial_j u_i)$$
...
$$\partial_t u_n = f_n(u_i, x_j, \partial_j u_i)$$
(1.1)

where i = 1, ..., k and j = 1, ..., m.

Discrete point symmetries are important for practical reasons. For example, they are used to increase the efficiency of numerical methods for solving differential equations; and are central to the development of many theories in physics such as quantum field theories. Given that the Lie symmetries of a system of differential equation exist, it is known how to generate all discrete symmetries of the system [9]. Otherwise, one has to solve a very complicated coupled nonlinear system of determining equations to identify the discrete symmetries. This is not always possible to do.

Here, we introduce a Mathematica code that generates, based only on algebraic calculations, a subset of the discrete symmetries of (1.1), namely, parity and permutation symmetries. A permutation symmetry is any permutation of the independent or dependent variables of (1.1) that leaves it unchanged. Similarly, a parity symmetry is any change in the sign of the independent or dependent variables of (1.1) that leaves it unchanged.

More specifically, our code generates the collection, Sym, of compound symme-

tries, defined by applying a permutation then parity transformation or vice versa. Since permutation and parity transformations do not always commute, one has to adapt an order convention for Sym.

Given a convention, we show that Sym forms a group. Groups are mathematical structures characterized, among others, by the closure of its elements under the associated operation. This property makes possible the generation of invariant quantities under such structures. Based on this result, we introduce a code that produces Sym-invariant polynomials, given any monomial. Indeed, these polynomials are conserved if the given monomial is conserved; this is because any symmetry of (1.1) maps conserved quantities to conserved quantities. We call this process symmetrization.

This thesis is structured in the following way. In chapter 2, we gather important mathematical results essential for this work. We assume the reader has knowledge of manifolds, differential forms, and vector fields. However, we introduce a quick introduction to these topics in Appendix A. In chapter 3, we review how Noether's theorem is used to connect variational symmetries to conserved quantities in Hamiltonian systems: this chapter contains only analytical methods. In chapter 4, we present our main results. This includes an algorithm for producing the group Sym, and another for producing the symmetrization of any list of monomials.

In this work, \mathbb{R}^d and \mathbb{C}^d stand for the real and complex d-th dimensional coordinate spaces, respectively. Other notations are always clearly defined as they are introduced. However, we clarify possible vagueness with the notations used for Schwartz and infinitely differentiable functions, denoted respectively by S and C^{∞} .

When these functions are defined on \mathbb{R}^d , we simply write $S(\mathbb{R}^d)$ and $C^{\infty}(\mathbb{R}^d)$. However, we sometimes work the nonrelativistic spacetime $\mathbb{R} \times \mathbb{R}^d$. In such cases, we want to be able to state a subdomain on which the property of the function applies, whether it is the time variable, space variables or both. To do this, we attach the following subscripts to the notation of the function class: the subscript x is used for space variables \mathbb{R}^d and t for the time variable \mathbb{R} . We also use loc to indicate that the property applies only locally. For example, $C_{t,loc}^{\infty}S_x(\mathbb{R}\times\mathbb{R}^d)$ indicates that the function is Schwartz (or rapidly decaying) with respect to space variables only, and that it is infinitely differentiable with respect to time locally.

Chapter 2

Mathematical Background

We lay the groundwork for this thesis by introducing fundamental concepts from symplectic geometry and group theory.

2.1 Symplectic geometry

In the Hamiltonian formulation of classical mechanics, a physical system is defined on a phase space that is equipped with a symplectic structure. The field concerned with such structures is called symplectic geometry. Here, we review relevant definitions and theorems from this field that we use in this work. We focus our attention on two phase spaces: differentiable manifolds and the space of square-integrable functions L^2 . We introduce the symplectic structure of the former here, but we limit our discussion of the latter to basic definitions; we introduce a particular symplectic structure associated with the phase space L^2 later when discussing the Schrödinger equation in chapter 3.

2.1.1 Symplectic manifolds

The main goal of this section is to develop the notion of a symplectic manifold. We start our discussion with the following definition.

Definition 2.1.1. A symplectic form is a closed nondegenerate 2-form.

Given a symplectic form, we define a symplectic manifold as follows.

Definition 2.1.2. Let M be a differentiable manifold and w be a symplectic form. A symplectic manifold is a pair (M, w), the manifold M equipped with a symplectic form w.

Next, we associate vector fields to scalar fields on (M, w) as follows.

Proposition 2.1.3. On (M, w), we uniquely define the Hamiltonian vector field of a smooth scalar field H, denoted by X_H , using the relation:

$$w(X_H, .) = dH(.).$$
 (2.1)

where dH is the exterior derivative of the scalar field H.

An important binary operation on scalar fields defined on (M, w) is the Poisson bracket.

Definition 2.1.4. Let M be a manifold and $F, G \in C^{\infty}(M \to \mathbb{R})$. The Poisson bracket $\{F, G\}$ is a binary operation with the following properties

• Bilinearity

$${F + G, H} = {F, H} + {G, H}$$
 and ${F, H + G} = {F, H} + {F, G}$;

• Skew-symmetry

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

• Jacobi identity

$${F, {H,G}} + {G, {F,H}} + {H, {G,F}};$$

• Leibniz rule

$$\left\{ FG,H\right\} =F\left\{ G,H\right\} +\left\{ F,H\right\} G.$$

We relate Poisson brackets to symplectic forms as follows.

Definition 2.1.5. On a symplectic manifold (M, w), we define the Poisson bracket associated with w as:

$$\{F,G\}(z) := w(z)(X_F(z), X_G(z)),$$
 (2.2)

where $F, G \in C^{\infty}(M \to \mathbb{R})$ with X_F and X_G being their corresponding Hamiltonian vector fields.

We introduce next a fundamental result to Hamiltonian mechanics.

Corollary 2.1.6. Let P be a Poisson manifold. Then,

$$\dot{F} = \{F, H\}$$
 for any smooth $F: P \to \mathbb{R}$.

where the relation only holds on the integral curves of X_H

Remark 2.1.7. We assume here that all scalar fields are not explicitly dependent on time.

Now, we introduce the definition of the Poisson bracket in canonical coordinates.

2.1.2 Function spaces as phase spaces

Here, we consider an important example of an infinite-dimensional phase space: $L^2(\mathbb{R}^d;\mathbb{C})$ (or $L^2(\mathbb{R}^d\to\mathbb{C})$).

L^2 space

Definition 2.1.8. We say $u \in L^2(\mathbb{R}^d; \mathbb{C})$ if and only if

$$L^{2}(\mathbb{R}^{d}; \mathbb{C}) = \left\{ u : \int_{\mathbb{R}^{d}} |u(x)|^{2} dx < \infty \right\}.$$

This function space comes equipped with the following inner product

$$\langle u, v \rangle = \int_{\mathbb{R}^d} u(x) \overline{v(x)} dx.$$

Definition 2.1.9. (Expectation values) Let A be a linear operator. The expectation value of A for a function u(x) is

$$E_u(A) = \langle Au, u \rangle.$$

For our purposes, we restrict the domain of A, D(A), to the following space:

Schwartz space

Definition 2.1.10. A function is u is Schwartz, if for all $\alpha, \beta \in \mathbb{N}^n$,

$$\sup_{x \in R^n} |x^{\beta} \partial^{\alpha} f(x)| < \infty.$$

We say that $u \in S(\mathbb{R}^n; \mathbb{C})$.

Remark 2.1.11. The set of smooth functions of compact support, $C_c^{\infty}(\mathbb{R}^n;\mathbb{C})$, is dense in $S(\mathbb{R}^n;\mathbb{C})$. This, in turn, means that $S(\mathbb{R}^n;\mathbb{C})$ is dense in $L^2(\mathbb{R}^n;\mathbb{C})$; this is because $C_c^{\infty}(\mathbb{R}^n;\mathbb{C})$ is dense in $L^2(\mathbb{R}^n;\mathbb{C})$. This property allows for a simpler treatment of the Schrödinger equation.

We end this section with the following definition.

Definition 2.1.12. (Bounded operators) An operator A bounded if $||A|| = \sup_{|u|=1} |Au|$ is finite.

2.2 Groups

We shift our attention to discussing another important mathematical structure: the group. We use this mathematical structure in Chapter 4 to develop our algorithms.

Definition 2.2.1. A set of elements G equipped with a binary operation * form an algebraic structure known as the group if it satisfies the following properties:

• Property 1 Closure:

If
$$g, f \in G$$
, then $g * f \in G$;

• Property 2 Identity:

Any group contains a unique element e such that for any $g \in G$, we have e * g = g * e = g. We call this element the identity element;

• Property 3 Inverse:

For every $g \in G$, there exists a unique element $k \in G$ such that k * g = g * k = e. We commonly write $k = g^{-1}$;

• Property 4 Associativity:

If
$$q, f, h \in G$$
, then $q * (f * h) = (q * f) * h$.

Remark 2.2.2. We can classify groups in terms of their order, the number of their elements. Under this classification, groups can be either finite or infinite.

2.2.1 Subgroups

We introduce the definition of a subgroup H of a group G.

Definition 2.2.3. Let G be a group, with an internal operation *, and H be a non-empty subset of G. H is a subgroup of G (H < G) if it satisfies

• Closure:

If $h, f \in H$, then $h * f \in H$;

• Inverse:

If $h \in H$, then $h^{-1} \in H$.

Definition 2.2.4. Let G be a group and let $T = \{t_1, t_2, ..., t_k\} \subseteq G$. The subgroup generated by T, denoted by $\langle T \rangle$, is the intersection of all subgroups $H \subseteq G$ such that $T \subseteq H$. Alternatively, define $T^{-1} = \{t_1^{-1}, t_2^{-1}, ..., t_k^{-1}\}$. Then, we write

$$\langle T \rangle = \left\{ a_1 * a_2 * \dots * a_n : n \in \mathbb{N} \text{ and } a_i \in T^{-1} \cup T \right\}.$$

We call the elements of T the generators of $\langle T \rangle$.

Example 2.2.5. Let $g \in G$. If $\langle g \rangle = G$, then G is called a cyclic group. In other words, any cyclic group G is generated by a single element g.

2.2.2 Direct products

Definition 2.2.6. Let $\{G_i\}_i = 1, 2, ..., N$ be a collection of groups. The direct product of $\{G_i\}$ is the cartesian product $G_1 \times ... \times G_N$. That is, the collection of all ordered N-tuples $(g_1, ..., g_N)$ such that $g_1 \in G_1, ..., g_N \in G_N$. Furthermore, the associated binary operation on the direct product is defined as:

$$(g_1,...,g_N)(h_1,...,h_N)=(g_1h_1,...,g_Nh_N).$$

Remark 2.2.7. The direct product always forms a group.

2.2.3 Group actions

Definition 2.2.8. Let G be a group and X be a set. A group action is a map $\alpha: G \times X \to X$ that satisfies

- $\alpha(e, x) = x$ for all $x \in X$;
- $\alpha(g, \alpha(f, x)) = \alpha(gf, x)$ for all $x \in X$ and $f, g \in G$.

2.2.4 Examples

The symmetric group S_n

Next, we discuss an important example of finite groups: the symmetric group. We start our discussion with an important, general remark about finite groups that we use repeatedly in chapter 4.

Remark 2.2.9. Let G be a finite group of order |G| and $g \in G$. Then, $g^n = e$ for some natural number $n \leq |G|$.

Now, we introduce the main definition.

Definition 2.2.10. The symmetric group of order n!, S_n , is the set of all permutations of any n-element set A. Let A be indexed by $\{1, 2, ..., n\}$. Then we write formally,

$$S_n = \{ \sigma : \{1, 2, ..., n\} \rightarrow \{1, 2, ..., n\} : \sigma \text{ is bijective.} \}.$$

Remark 2.2.11. The following notation is commonly used to represent any element of S_n

$$\left(\begin{array}{cccc}
1 & 2 & \dots & n \\
\sigma(1) & \sigma(2) & \dots & \sigma(n)
\end{array}\right)$$

Example 2.2.12. The element of S_3 defined by the bijection,

$$\sigma(1) = 1$$

$$\sigma(2) = 3$$

$$\sigma(3) = 2$$

can be denoted by

$$\left(\begin{array}{ccc} 1 & 2 & 3 \\ & & \\ 1 & 3 & 2 \end{array}\right)$$

Definition 2.2.13. A compact way of describing a permutation is **the cyclic notation**. To describe any permutation σ , we write it in the following form:

$$\sigma = (k_1, k_2, ..., k_r).$$

Here, $\{k_1, k_2, ..., k_r\} \subset \{1, 2, ..., n\}$ for some $r \leq n$ such that:

$$\sigma(k_i) = k_{i+1} \quad 1 \leqslant i \leqslant r - 1$$

 $\sigma(k_r) = k_1$

 $\sigma(k) = k$ Otherwise

Example 2.2.14. The element in example 2.2.12 can be written as $\sigma = (23)$.

Remark 2.2.15. Given a finite set X, the permutations of elements of X define a group whose action on X is permutations themselves. The group action is then naturally defined; we usually don't distinguish between the group and its action in such cases. However, not all groups have a naturally defined action. In such cases, the distinction becomes clear.

Lie Groups

We can impose on any group additional mathematical structures. For example, we can impose a topological structure. This type of group is called a topological group. We are not interested in rigorously developing the notion of topological groups. However, we mention here an important example: the Lie group.

A Lie group is an n-dimensional smooth and real manifold that also satisfies, under some binary operation, the properties of a group. Here, we present a specific type of Lie group that is of interest to us, namely, the one-parameter unitary group.

Definition 2.2.16. (One-parameter unitary groups) A one-parameter unitary group A(t) is a set of bounded linear operators satisfying:

- |A(t)u| = |u| (unitary operators);
- A(0) = id;
- A(t+s) = A(t)A(s).

We define the infinitesimal generator H of such a group in the following way:

$$Hu = \lim_{t \to 0} \frac{i\hbar}{t} (A(t)u - u),$$

$$D(H) = \{ u \in L^2(\mathbb{R}^d; \mathbb{C}) : Hu \text{ exists} \}.$$

Example 2.2.17. The one-parameter unitary group of time translations U(t) defined by $U(t)u_0(x) = u(x,t)$ has the infinitesimal generator $i\hbar \frac{d}{dt}$ if $u_0(x) \in L^2(\mathbb{R}^d;\mathbb{C})$. Then, $i\hbar \frac{d}{dt}u(x,t) = Hu$. This is known as **the Schrodinger equation** (associated with the Hamiltonian H). Its solution can be written as $u(x,t) = e^{-iHt/\hbar}u(x,0)$.

2.3 Invariance and conservation laws

A central theme in this work is the connection between invariance and conservation laws. Here, we introduce concepts that we use to investigate this connection in chapter 3 and 4, namely, symmetries and conservation laws.

2.3.1 Symmetries

Definition 2.3.1. Symmetries are transformations that leave the object they act on unchanged.

Remark 2.3.2. This definition is very general. We introduce more specific definitions as needed.

A useful set of transformations can be defined based on the nature of the domain on which they act. In this sense, we can classify symmetries as continuous or discrete. **Continuous symmetries** are transformations that are functions of continuous parameters. That is, they are associated with a continuous change of the shape of the object they act on. Similarly, we say that **discrete symmetries** are functions of parameters that are discrete, thereby changing the object they act on in discrete units. Examples of symmetries include, but not limited to,

• Rotations

A rotational symmetry is any transformation of an object around a fixed point that leaves the object unchanged. Famously, the circle has a rotational continuous symmetry about its center at any angle. An equilateral triangle has a rotational discrete symmetry about its center: rotations of 60, 120 and 180 degrees. We call the number of possible degrees the **order of the rotational** symmetry. Thus, a circle has a symmetry of order ∞ while an equilateral triangle's symmetry is of order 3.

Scalings

A scale symmetry is a transformation which rescales the object it acts on in such a way it leaves it unchanged. For example, if u(x,t) is a classical solution to a certain PDE, then a transformation

$$u(x,t) \to \lambda^k u(\lambda^n x, \lambda^m t).$$

is a scale symmetry if it is a solution to the PDE for some given k,n,m.

Translations

A translational symmetry is any translation that leaves a system invariant. An example can be seen in classical Hamiltonian systems. Such systems are invariant under translations in time. Formally, one would say

$$u(x,t) \to u(x,t+\Delta t)$$
.

is always a solution to any Hamiltonian system if and only if u(x,t) is a solution.

Some symmetries are necessarily non-continuous transformations. Reflections of objects or permutations of the independent/dependent variables of a dynamical system are examples of such category.

• Reflections

Reflectional symmetry is closely related to rotational symmetry. A reflectional symmetry is a distance-preserving mapping across a hyperplane, a line for example, that doesn't change the shape of the object it acted on. An example of such symmetry is that of a reflection of a circle across any line passing through its center.

Remark 2.3.3. Every rotation can be thought of as a set consecutive reflections.

• Permutations

Let D be the ordered set of variables of a system of PDEs. A permutation symmetry is a permutation of D that leave the system unchanged. We elaborate on this type of symmetries in chapter 4.

2.3.2 Conservation laws

In time-dependent systems of PDEs, a conserved quantity is a function f(t) of the dependent variables such that its time derivative is zero. Commonly, f(t) is an integral

of some density function, u(x,t), over a region V. That is, $f(t) = \int_V u(x,t) dx$. In such cases, one can show that there exists a local conservation law associated with this quantity. Mathematically, local conservation laws are written in the following form:

$$\partial_t u(x,t) = \nabla \cdot J,$$

where J is a function representing the flux of u(x,t). This form is known as the differential form of continuity equations.

Chapter 3

Symmetries and Conservation laws in Hamiltonian Systems

In this chapter, we investigate symmetries and conservation laws using analytical methods. We apply the the theory presented in chapter 2 to two types of systems: a classical particle in a scalar potential field and a free quantum particle. These systems are described using Newton's laws and the free Schrödinger. We use the Hamiltonian formulation to derive our results. The central goal of this chapter is to introduce Noether's theorem, and how it is used to connect continuous symmetries to conservation laws.

3.1 Newtonian mechanics

We discuss here the case of a single point particle of mass m moving in a potential field V. A natural setting for such systems is finite-dimensional real symplectic vector spaces. We define first such vector spaces. Then, we use this mathematical structure to reproduce Newton's second law, a conservation law for linear momentum in conservative systems.

3.1.1 Symplectic vector spaces

We assume the reader is familiar with the definition of real, n-dimensional vector spaces, commonly denoted by \mathbb{R}^n , which is also a manifold. We know from chapter 2 that a symplectic manifold is a pair (M, w). Since we work with \mathbb{R}^n , we introduce a special definition of symplectic forms on real, finite dimensional vector spaces. We

choose the notation B instead of w to denote them.

Definition 3.1.1. Let \mathbb{K} be a field of scalars and E be an n-dimensional real vector space. A symplectic form B is a mapping $B: E \times E \to \mathbb{K}$ with the following properties,

• Bilinear:

A bilinear form is linear in both arguments separately, over the field of scalars \mathbb{K} .

• Anti-symmetric:

For $u, v \in E$, we have B(u, v) = -B(v, u).

• Non-degenerate:

For every nonzero $u \in E$, there exists a vector v such that $B(u, v) \neq 0$. Alternatively, if B(u, v) = 0 for all $v \in E$, then u = 0.

Remark 3.1.2. This definition is a special case of definition 2.1.1.

We are now ready to present the definition of symplectic vector spaces,

Definition 3.1.3. A symplectic vector space is a finite-dimensional vector space E, over \mathbb{K} , equipped with a symplectic form B. We use the notation (E, B) to denote this vector space.

Next, we define important operations on symplectic vector spaces vector spaces,

• 1) The symplectic gradient:

Definition 3.1.4. The symplectic gradient of a function $P \in C^1_{loc}(E \to \mathbb{R})$ is the endomorphism $\nabla_B P \in C^0_{loc}(E \to E)$ defined such that:

$$\frac{d}{d\epsilon}P(u+\epsilon v)|_{\epsilon=0} = B(\nabla_B P(u), v). \tag{3.1}$$

Claim 1. This gradient is unique due the non-degeneracy of the symplectic form.

Proof. Assume, to the contrary, that there exists another gradient $\overline{\nabla}_B P$ that satisfies the relation above. Then,

$$B(\nabla_B P, v) = B(\overline{\nabla_B P}, v).$$

By the bilinearity, it follows that:

$$B(\nabla_B P - \overline{\nabla_B P}, v) = 0.$$

The uniqueness follows then from the nondegenracy of B

$$\nabla_B P - \overline{\nabla}_B P = 0 \implies \nabla_B P = \overline{\nabla}_B P.$$

Remark 3.1.5. Equation (3.1) is a special case of equation (2.1). That is, the symplectic gradient of P, $\nabla_B P$, is the Hamiltonian vector field X_P defined within this context.

• 2) The Poisson bracket

Definition 3.1.6. The Poisson bracket is an operation defined on any $P,Q \in C^1_{loc}(E \to \mathbb{R})$ as follows:

$$\{P,Q\}(u) = B(\nabla_B P(u), \nabla_B Q(u)). \tag{3.2}$$

• 3) The Hamiltonian

Definition 3.1.7. A function $H \in C^2_{loc}(E \to \mathbb{R})$ is called a Hamiltonian.

Remark 3.1.8. This Hamiltonian is a fundamental quantity in the Hamiltonian formulation of mechanics; it is the total energy of a Hamiltonian system.

Using the Hamiltonian, we define the Hamiltonian flow.

Definition 3.1.9. The Hamiltonian flow of a Hamiltonian H is given by the integral curves of the ODE

$$\frac{\partial u(t)}{\partial t} = \nabla_B H(u(t)). \tag{3.3}$$

Finally, we introduce a specific version of Noether's theorem to symplectic vector spaces.

Theorem 3.1.10. (Noether's theorem) Assume that u, v are classical solutions of the Hamiltonian flows of two Hamiltonians H, P, respectively. Then, the following statements are equivalent:

- H and P Poisson commute. That is, $\{P, H\} = \{H, P\} = 0$;
- P(u(t)) is constant;
- H(v(t)) is constant.

Before we prove the theorem, we introduce the following lemma

Lemma 3.1.11. Let P, H, u and v be defined as in theorem 3.1.10. Then,

$$\frac{\partial P(u(t))}{\partial t} = \{P, H\}.$$

Similarly,

$$\frac{\partial H(v(t))}{\partial t} = \{H, P\}.$$

Proof. (of lemma 3.1.11)

By equations 3.1, 3.2 and 3.3, we have

$$\begin{split} \frac{dP(u(t))}{dt} &= \frac{dP}{du_1} \frac{du_1}{dt} + \ldots + \frac{dP}{du_n} \frac{du_n}{dt} = \frac{d}{d\epsilon} P(u + \epsilon \frac{du}{dt})|_{\epsilon=0} \\ &= B(\nabla_B P(u), \frac{du}{dt}) = B(\nabla_B P(u), \nabla_B H(u)) = \{P, H\} \,. \\ \frac{dH(v(t))}{dt} &= \frac{dH}{dv_1} \frac{dv_1}{dt} + \ldots + \frac{dH}{dv_n} \frac{dv_n}{dt} = \frac{d}{d\epsilon} H(v + \epsilon \frac{dv}{dt})|_{\epsilon=0} \\ &= B(\nabla_B H(v), \frac{dv}{dt}) = B(\nabla_B H(v), \nabla_B P(v)) = \{H, P\} \,. \end{split}$$

Proof. (of theorem 3.1.10) The proof is obvious using lemma 3.1.11 except for the the statement:

$$\{P, H\} = 0 \iff \{P, H\} = \{H, P\}.$$

The proof for this is as follows. If $\{P, H\} = \{H, P\}$, then by definition (3.2) $B(\nabla_B P(u), \nabla_B H(u)) = B(\nabla_B H(u), \nabla_B P(u))$. By the antisymmetry of B, it follows that $B(\nabla_B P(u), \nabla_B H(u)) = -B(\nabla_B P(u), \nabla_B H(u))$. Thus, $B(\nabla_B P(u), \nabla_B H(u)) = \{P, H\} = \{H, P\} = 0$. The other direction is trivial.

A different interpretation of Noether's theorem is given by the next proposition

Proposition 3.1.12. Denote by $\alpha_P(t)$ the flow maps of P and assume they are globally defined, e.g., when $\nabla^2 P$ is bounded. Then, P is a conserved quantity for equation (3.3) if and only if H is invariant under the action of the flow maps $\alpha_P(t)$.

Proof. If H is invariant under the action of $\alpha_P(t)$, then H(v(t)) is constant. Then it follows, by theorem (3.1.10), that P(u(t)) is conserved. Similarly, if P(u(t)) is conserved, then H(v(t)) is conserved.

Remark 3.1.13. The flow maps $\alpha_P(t)$, defined as in (3.1.12), have the following properties: S(0)=Id and S(t+t')=S(t)S(t'). The condition that $\nabla^2 P$ is bounded ensures that $\alpha_P(t)$ is defined for any $t \in \mathbb{R}$; it is then easy to check that they form a group. Furthermore, $\alpha_P(t)$ are diffeomorphisms.

Example 3.1.14. Consider the Hamiltonian $P(z) = \frac{1}{4}|z|^4$ with the associated (complex scalar) Hamiltonian ODE

$$\dot{z} = i|z|^2 z.$$

The flow maps $\alpha_P(t)$ act on the complex plane by rotating every point in circular fashion; this is because the general solution is $z(t) = z(0)e^{i(z(0))^2t}$. Thus, the quantity $H(z) = |z|^2$ is invariant by the action of $\alpha_P(t)$. It follows by proposition (3.1.12) that P is conserved by the Hamiltonian flow of H.

3.1.2 The second law of motion

We now show how to recover Newton's second law for a point particle of mass m in a potential field V. We first introduce the following vector space.

$$E = \mathbb{R}^n \times \mathbb{R}^n = \{ (\vec{q}, \vec{p}) = (q_1, ..., q_n, p_1, ..., p_n) : q_i, p_i \in \mathbb{R}, 1 \le i \le n \}.$$
 (3.4)

Remark 3.1.15. This is the cotangent bundle of \mathbb{R}^n .

On E, we introduce the canonical definitions:

• The symplectic form

$$B((q_1, ..., q_n, p_1, ..., p_n), (q'_1, ..., q'_n, p'_1, ..., p'_n)) = \sum_{i=1}^n q_i p'_i - q'_i p_i.$$

• The symplectic gradient

For $H, P \in C^1_{loc}(E \to \mathbb{R})$, the symplectic gradient is as follows

$$\nabla_B H = \left(\frac{\partial H}{\partial p_1}, ..., \frac{\partial H}{\partial p_n}, \frac{-\partial H}{\partial q_1}, ..., \frac{-\partial H}{\partial q_n}\right).$$

• The Poisson Bracket

$$\{P, H\} = \sum_{i=1}^{n} \frac{\partial H}{\partial p_i} \frac{\partial P}{\partial q_i} - \frac{\partial H}{\partial q_i} \frac{\partial P}{\partial p_i}.$$

Remark 3.1.16. This choice of this specific vector space as well as the above operations is driven by our knowledge the Lagrangian formalism of mechanics. We omit discussing this issue here. However, we note that the q_i 's and the p_i 's are commonly referred to as generalized coordinates and momenta of the particle, respectively.

Now, for a generic Hamiltonian H, we have the following flow of H,

$$\frac{\partial}{\partial t}(q_1, ..., q_n, p_1, ..., p_n) = \left(\frac{\partial H}{\partial p_1}, ..., \frac{\partial H}{\partial p_n}, \frac{-\partial H}{\partial q_1}, ..., \frac{-\partial H}{\partial q_n}\right). \tag{3.5}$$

Remark 3.1.17. The system of ODEs (3.5) is commonly known as Hamilton's equations

If we define our Hamiltonian to be,

$$H = \frac{1}{2m} |\vec{p}|^2 + V(\vec{q}),$$

where $V(q) \in C^2_{loc}(\mathbb{R}^n \to \mathbb{R})$. Then it follows that

$$\begin{cases}
 m \frac{\partial}{\partial t} \vec{q}(t) &= \vec{p}(t) \\
 \frac{\partial}{\partial t} \vec{p}(t) &= -\nabla V(\vec{q}(t)).
\end{cases}$$
(3.6)

Remark 3.1.18. The first equation is the definition of the momentum while the second equation is Newton's Second Law for conservative systems.

Finally, we discuss some applications of Noether's theorem. It is clear that the Hamiltonian H Poisson commutes with itself. Thus, the quantity H(q, p) is conserved along the integral curves of the Hamiltonian flow. This is a statement of the conser-

vation of energy since the Hamiltonian represents the total energy of the particle.

If we set V(q) = V, we have a Hamiltonian H that is invariant under spatial translations. In this case, we see that the total momentum |p| Poisson commutes with H. This is a statement of the conversation of momentum. Similarly, if V(q) is invariant under rotations, H becomes invariant under rotational translations. Here, the angular momentum $L = q \times p$ poisson commutes with H, thereby implying the conservation of angular momentum.

3.2 The Schrödinger equation

An example of a Hamiltonian PDE is the Schrödinger equation. This equation is fundamental to our understanding of the quantum world. Its importance, however, goes beyond quantum mechanics. The Schrödinger equation belongs to a class of PDEs known as constant-coefficient linear dispersive (CCLD) PDEs. This class of PDEs has application to several fields such as geometry, spectral theory and number theory [1]. Here, we focus on the conservation laws and symmetries of the Schrödinger equation in the hope of gaining a general understanding on how conservation laws and symmetries arise in Hamiltonian PDEs. We start with a quick introduction to CCLD PDEs.

Definition 3.2.1. Let L be the operator defined as,

$$Lu(x) = \sum_{|\alpha| \le k} c_{\alpha} \partial_x^{\alpha} u(x).$$

Given $u_0(x) = u(0, x)$, a constant-coefficient linear dispersive PDE has the following form:

$$\partial_t u(t, x) = Lu(t, x), \tag{3.7}$$

where $u: \mathbb{R} \times \mathbb{R}^d \to \mathbf{V}$, \mathbf{V} a vector space.

Remark 3.2.2. The operator ∂_x^{α} is defined in the standard way for classical solutions and L is skew-adjoint. Also, let $End(\mathbf{V})$ indicates the space of all linear transformation from \mathbf{V} to \mathbf{V} . Then, $c_{\alpha} \in End(\mathbf{V})$ are coefficients that define the dispersion relation $h(k_1, ..., k_d) = \sum_{|\alpha| \leq k} i^{|\alpha|-1} c_{\alpha} k_1^{\alpha_1} ... k_d^{\alpha_d}$. This is done by letting L = ih(D) where $D = \frac{1}{i} \nabla$.

Now, we are ready to present the Schrödinger equation

Definition 3.2.3. (The Schrödinger equation) Let Δ be the Laplacian. Setting $L = \frac{i\hbar}{2m}\Delta$, we retrieve the free Schrödinger equation,

$$\partial_t u = \frac{i\hbar}{2m} \Delta u.$$

Remark 3.2.4. Here, $u: \mathbb{R} \times \mathbb{R}^d \to \mathbf{V}$ is a complex vector field and the dispersion relation is $h(k_1, ..., k_d) = -\frac{\hbar}{2m} \sum_{i=1}^d k_i^2$. Also, the operator $H = \frac{\hbar}{2m} \Delta$ is commonly referred to as the Hamiltonian operator for a free quantum particle.

Proposition 3.2.5. Let $L^2(\mathbb{R}^d;\mathbb{C})$ be equipped with a symplectic form $B(u,v) = -2\int_{\mathbb{R}^d} Im(u(x)\overline{v(x)})dx$. Then, the Schrodinger equation is the Hamiltonian flow associated with the densely defined Hamiltonian $P(u) = \frac{\hbar}{2m}\int_{\mathbb{R}^d} |\nabla u|^2 dx$.

Proof.

$$\frac{d}{d\epsilon}P(u+\epsilon v)|_{\epsilon=0} = \frac{\hbar}{2m} \int_{\mathbb{R}^d} \frac{du}{dx_i} \frac{\overline{dv}}{dx_i} + \frac{dv}{dx_i} \frac{\overline{du}}{dx_i}$$

$$= \frac{-\hbar}{2m} \int_{\mathbb{R}^d} \frac{d^2u}{dx_i^2} \overline{v} + v \frac{\overline{d^2u}}{dx_i^2}$$

$$= \frac{-\hbar}{2m} \int_{\mathbb{R}^d} 2Im(iv \frac{\overline{d^2u}}{dx_i^2})$$

$$= -2 \int_{\mathbb{R}^d} Im(\overline{-\frac{i\hbar}{2m}} \frac{d^2u}{dx_i^2} v)$$

$$= B(v, \frac{-i\hbar}{2m} \frac{d^2u}{dx_i^2}) = B(\frac{i\hbar}{2m} \frac{d^2u}{dx_i^2}, v).$$

Thus, the associated Hamiltonian flow is:

$$\partial_t u = \frac{i\hbar}{2m} \Delta u. \tag{3.8}$$

To learn about the conservation laws in the Schrödinger equation, we introduce the Heisenberg equation. This equation describes the dynamics of a quantum free particle in terms of Lie brackets.

Proposition 3.2.6. (Heisenberg equation) Let $u \in C_t^{\infty} S_x(\mathbb{R} \times \mathbb{R}^d)$ be a classical solution of equation (3.8) and A be a time-independent continuous linear operator $S(\mathbb{R}^d) \to S(\mathbb{R}^d)$. Then,

$$\frac{d}{dt}\langle Au(t), u(t)\rangle = \langle \frac{i}{\hbar}[H, A]u(t), u(t)\rangle,$$

where [H, A] = HA - AH, the Lie Bracket.

Remark 3.2.7. The Heisenberg equation is the quantum analogous to lemma (3.1.11);

the connection between Poisson and Lie brackets can be established using semiclassical analysis tools.

We omit the proof for proposition (3.2.6) as it is beyond the scope of this work. Instead, we introduce Noether's theorem for the free Schrödinger equation.

Theorem 3.2.8. (Noether's theorem) Let A be defined as in proposition (3.2.6) such that [H, A] = [A, H] = 0. Then, A is a conserved quantity and D(A) is invariant under the action of the unitary group $U(t) = e^{-itH/\hbar}$. That is,

$$\langle Au(t), u(t) \rangle = \langle Au(0), u(0) \rangle;$$

$$u(t) = e^{-itH/\hbar}u(0) \in D(A)$$

Proof. The first statement follows directly from proposition (3.2.6). The proof for the second statement is beyond the scope of this work.

Remark 3.2.9. $e^{-iHt/\hbar}$ is a one-parameter, t, Lie group.

Let $u \in C^{\infty}_{t,loc}S_x(\mathbb{R} \times \mathbb{R}^d)$. Then, the Schrödinger equation has following symmetries and conservation laws:

• Space and time symmetries

(Invariance under time translations)

$$u(x,t) \rightarrow u(x,t-t_0).$$

The generator the one-parameter group of time translations is the Hamiltonian operator H. Clearly, H commutes with itself. Thus, $\langle Hu(t), u(t) \rangle = \int_{\mathbb{R}^d} \overline{u(x,t)} Hu(x,t) dx = \frac{\hbar}{2m} \int_{\mathbb{R}^d} |\nabla u(x,t)|^2 dx$ is conserved.

(Invariance under spatial translations)

$$u(x,t) \rightarrow u(x-x_0,t).$$

The generator for the one-parameter group of translations is $p_j = \frac{1}{i}\nabla_j$. Indeed, $[H, p_j] = 0$, and thus $\int_{\mathbb{R}^d} \overline{u(x,t)} p_j u(x,t) dx = \int_{\mathbb{R}^d} Im(\overline{u(x,t)} \frac{d}{dx_j} u(x,t)) dx$ is conserved. Consequently, the vector-valued function $\vec{P} = (p_1, ..., p_d)$ is conserved. Furthermore, $u(t) = e^{-itH}u(0) \in D(p_j) = C_t^{\infty} S_x(\mathbb{R} \times \mathbb{R}^d)$

• Phase rotation symmetry

$$u(x,t) \to e^{i\theta} u(x,t).$$

The related conserved quantity is $\int_{\mathbb{R}^d} |u(x,t)|^2 dx$.

• Galilean symmetry

Let $u \in C^2_{loc}(\mathbb{R} \times \mathbb{R}^d \to \mathbf{V})$ (a complex field). Then, an interesting symmetry of the Schrodinger equation is

$$u(x,t) \to \tilde{u}(x,t) = e^{\frac{imxv}{\hbar}} e^{\frac{imt|v|^2}{2\hbar}} u(x-vt,t).$$

with $v \in \mathbb{R}^d$ and $\tilde{u} \in C^2_{loc}(\mathbb{R} \times \mathbb{R}^d \to \mathbb{C})$. The related conserved quantity is the normalized center of mass $\int_{\mathbb{R}^d} x |u(x,t)|^2 dx - t\vec{P}$.

The Schrödinger equation also has the following discrete symmetries.

• Time-reversal symmetry

The Schrödinger equation is invariant under an inversion of time and space coordinates. That is, it has the symmetry,

$$u(x,t) = u(-x,-t).$$

• Scaling symmetry

The transformation

$$u(x,t) \to u\left(\frac{t}{\lambda^2}, \frac{x}{\lambda}\right).$$

is a symmetry of the Schrödinger equation. In general, if $P: \mathbb{R}^d \to \mathbb{C}$ is a homogeneous kth degree polynomial and $L = P(\nabla)$, then equation (3.7) has the symmetry

$$u(x,t) \to u\left(\frac{t}{\lambda^k}, \frac{x}{\lambda}\right).$$

Chapter 4

The Symbolic Computational Approach

The primary focus of this work is to introduce symbolic computational methods for detecting parity and permutation symmetries as well as for generating new conserved quantities from known conserved quantities. Symbolic computations are algebraic manipulations of expressions. In this chapter, we introduce the mechanics of such computations as well as algorithms for specific cases. This includes necessary mathematical proofs and Mathematica codes.

4.1 Overview

Recall from previous chapters that Noether's theorem allows us to use groups to identify conserved quantities in PDE systems admitting a variational principle. More specifically, each Hamiltonian defines a Lie group of time-evolution operators acting on phase space, defining the Hamiltonian flow; then the invariance of a quantity under the action of this group implies its conservation. Given a symplectic structure, checking for conserved quantities can be done through binary operations such as Poisson and Lie brackets.

For general evolution equations, these results don't always hold. Indeed, we don't necessarily have a Hamiltonian flow with an associated Lie group. However, it is always true that a symmetry of a system of differential equations maps a conserved quantity to another conserved quantity. Hence, one can generate new conserved quantities from known ones using any symmetry. Here, we focus only on generating

conserved quantities using groups of symmetries. We call this process symmetrization. This allows us to use elements from group theory to construct more complex algorithms as we shall see in this chapter. Before we examine the concept of symmetrization closely, we introduce an important tool: the master polynomial.

4.1.1 The master polynomial

Assume P and G are a conserved quantity and a group of symmetries, respectively, for the following (standard) system:

$$\partial_t u_1 = f_1(u_i, x_j, \partial_j u_i)$$

$$\partial_t u_2 = f_2(u_i, x_j, \partial_j u_i)$$

$$\partial_t u_3 = f_3(u_i, x_j, \partial_j u_i)$$
...
$$\partial_t u_n = f_n(u_i, x_j, \partial_j u_i).$$
(4.1)

where i = 1, ..., k and j = 1, ..., m.

We can generate a new conserved quantity P' as follows. We apply each symmetry in G to P, and then sum up all these elements. Thus, P' can be a finite or infinite sum, depending on the size of G. Because there is no general theory for systems of the form (4.1), it is not obvious whether this sum is well-defined. Here, we show that it is indeed well-defined using the concept of a master polynomial.

The master polynomial is a formal series of all possible monomials in the dependent variables of the system and derivatives thereof. Then, this polynomial includes all possible choices for P'. It then suffices to show that the master polynomial is well-defined. Specifically, we want to show that the sum can be indexed by a countable set.

For a system of differential equations with k independent variables $\vec{x} = (x_1, ..., x_k)$

and m dependent variables $\vec{u} = (u_1(t, x_1, ..., x_k), ..., u_m(t, x_1, ..., x_k))$, we consider the two sets:

• The set $\{h_j\}_{j=1,2...}$ with the ith element defined as

$$h_i = u_1^{a_{10}} (\partial_1 u_1)^{a_{11}} ... (\partial_k u_1)^{a_{1k}} ... u_m^{a_{m0}} (\partial_1 u_m)^{a_{m1}} ... (\partial_k u_m)^{a_{mk}},$$

for some $\vec{a_i} = (a_{10}, ..., a_{1k}, a_{20}...a_{2k}..., a_{m0}, ...a_{mk})$ with $a_{ij} \in N \cup \{0\}$

• The set $\{c_j\}_{j=1,2...}$ of unknown constants.

Claim 2. $\{h_j\}$ is countable.

Proof. Every element of $\{h_j\}$ is associated with an element from the set K containing the vectors $\vec{a} = (a_{10}, ..., a_{1k}, a_{20}...a_{2k}..., a_{m0}, ...a_{mk})$. The set K is countable. This is just an extension of the result that integers are countable to arbitrary (mk)-tuples of nonnegative integers.

Remark 4.1.1. The set $\{h_j\}$ is the set of all possible monomials in the dependent variables and their derivatives. For example, $(u_1)^2(d_1u_1)^3$ is the element associated with the vector $\vec{a_i} = (2, 3, 0, ..., 0)$.

Definition 4.1.2. The master polynomial is the formal series

$$f = \sum_{j \in \mathbb{N}} c_j h_j. \tag{4.2}$$

This polynomial is determined by the two sets $\{h_j\}_{j=1,2...}$ and $\{c_j\}_{j=1,2...}$.

Remark 4.1.3. Claim 2 justifies our choice of indexing the set $\{h_j\}$ by the natural numbers, that is, it justifies the formal series.

4.1.2 The symmetrization process

An introductory example

Example 4.1.4. Consider the following system:

$$v_t = u$$

$$u_t = -v.$$
(4.3)

An apparent symmetry of this system is the following:

$$(u,v) \to (v,-u).$$

It is easy to check that this symmetry together with the identity symmetry form a group. Now, consider the polynomial defined by $\{h_j\}_{j=1,2} = \{u^2\}$ and $\{h_j\}_{j=2,3,4,...} = 0$. That is,

$$f(u,v) = c_1 u^2.$$

Applying the two symmetries in the previous group, and summing produces the polynomial

$$\overline{f}(u,v) = c_1(u^2 + v^2).$$

Differentiating with respect to time gives

$$\overline{f}_t = c_1(2uu_t + 2vv_t) = c_1(-2uv + 2vu) = 0.$$

Thus, we managed to deduce that f(u, v) is a conserved quantity. Indeed, we can double-check this result by solving equation (4.3) directly. The solution is:

$$u = A\cos(t + \theta_0)$$
 and $v = A\sin(t + \theta_0)$.

whose trajectory moves on a circle of origin zero with a fixed radius, the conserved quantity.

Note that the choice of u^2 is deliberate. We could have worked instead with the polynomial

$$f(u, v, u_t, v_t) = c_1 u^2 + c_2 v^2 + c_3 u_t v_t + c_4 u_t^2.$$

However, this choice would not have helped us with extracting additional information about the conserved quantities in the system. This suggests that our understanding of the nature of the system is essential in the construction of a useful truncated master polynomial. Indeed, with additional information, we can approach the problem in a more focused and structured way.

Symmetrization of monomials

Assume now we have, for our system of PDEs, a group G of its discrete symmetries. Then, we define the symmetrization of any element as follows

Definition 4.1.5. Let G be a group of discrete symmetries for a system of PDEs. A symmetrization of an element $x \in \{h_j\}_{j=1,2...}$ with respect to G is the sum $\beta_G(x)$ associated with the group action $\beta(g,x)$; it is defined as:

$$\beta_G(x) = \frac{1}{|G|} \sum_{g \in G} \beta(g, x).$$

This defines a possible truncated master polynomial.

The process of finding possible conserved quantities then is as follows. We identify a group G of discrete symmetries for the system. Then, we choose an element $x \in \{h_j\}_{j=1,2...}$ to create a candidate conserved quantity $\beta_G(x)$. To check if it is conserved, we simply differentiate with respect to time. Indeed, we know it is conserved if the element x is conserved.

To make use of this method, one has to identify first at least one or more groups of discrete symmetries. However, symmetries are not always obvious to spot. We devote the next section to discussing specific methods to finding such groups.

4.2 Analysis of specific symbolic algorithms

We focus our attention here on specific discrete symmetries that we can deal explicitly with; specifically, we introduce symbolic algorithms to compute permutation and parity symmetries in systems of PDEs.

Permutation symmetries

Consider a system of PDEs given in the standard form given by (4.1). We are interested in examining how shuffling around the variables of this system affects the system itself. We start with some necessary definitions

Definition 4.2.1. A permutation is a map

$$(u_1,..,u_k,x_1,...,x_m) \to P(u_1,..,u_k,x_1,...,x_m)$$

that rearranges the variables in a new order. P is called the permutation operator.

We wish to distinguish between a permutation operator acting on the dependent variables and one acting on the independent ones. We denote the first with P_d and the latter with P_I . Compactly, we write P_r with $r \in \{I, d\}$

Now, we are in a position to define a permutation symmetry.

Definition 4.2.2. A permutation symmetry is a map

$$(u_1,..,u_k,x_1,...,x_m) \to P_r^s(u_1,..,u_k,x_1,...,x_m)$$

such that the system (4.1) is left unchanged up to a reordering of the equations.

Theorem 4.2.3. Let $(r,t) \in \{(I,m),(d,k)\}$ be fixed. Also, let $X_d = \{u_1,...,u_k\}$, $X_I = \{x_1,...,x_m\}$ and S_t be the symmetric group of order t. The set of maps P_r of (4.1) are naturally defined by the group action $\alpha_r : S_t \times X_r \to X_r$. Similarly, the set of maps P_r^s of (1.1) are naturally defined by the group action $\alpha_r^s : O_r \times X_r \to X_r$, where $O_I < S_m$ and $O_d < S_k$.

Proof. We want to prove the claim that $O_r < S_t$. Note that any permutation symmetry is a permutation transformation. It then suffices to show that elements of O_r have the two properties: (1) They are closed under the naturally defined operation; (2) and for each permutation $o \in O_r$, $o^{-1} \in O_r$.

Statement (1) is true because the application of two different permutations, each of which leaving the system (1.1) unchanged, leaves it unchanged. Statement (2) follows because O_r is finite, and thus it must be that $o^k = Id$ for some $k \in \mathbb{N}$, thereby implying that $oo^{k-1} = Id$, and consequently that $o^{k-1} = o^{-1}$. Therefore, by statement (1), we have $o^{-1} \in O_r$.

Next, we define permutation-invariant systems.

Definition 4.2.4. A system is permutation-invariant if all the possible k+m permutations are permutation symmetries of that system. In other words, it is permutation-invariant if $|G_d| + |G_I| = k + m$.

Now, we explore the problem of symbolically identifying permutation symmetries systems of standard form. If we assume the number of variables to be small enough, which is a statement dependent on the computational power available, we can use the following algorithm to identify the permutation symmetries. We begin with an algorithm that identifies the group G_d .

4.2.1 Algorithm I

As it is going to be the case throughout this thesis, all codes will be Mathematica codes. The first code is as follows:

The function F has three variables. The variable expres is a list of the PDEs in the systems. The variables depVars and IndVars are lists of the dependent variables and independent variables, respectively. Note that the system has to be rewritten in the same format as in (4.1) before inputting the variables.

Example 4.2.5. As an example, consider the system

$$\dot{u} - u + v = 0$$

$$\dot{v} + u - v = 0.$$

We see that the non-trivial and trivial permutations $P_1(u,v) = (u,v)$ and $P_2(u,v) = (v,u)$ are all permutation symmetries. Furthermore, $|S_2| = 2$. When we run the code above and then run the following line

$$F \ [\{D[v[t], t] - v + u, D[u[t], t] - u + v\}, \{u, v\}, \{t\}]$$

The code outputs *True* to confirm that the system is permutation-invariant. A *False* output would indicate otherwise. We then run the following line

PermutationGroup[Map[FindPermutation, p]]//GroupGenerators

In light of Theorem (4.2.3), this line of the code outputs the generators of the associated symmetric group, $S_{|G_d|}$. In this example, it happens that all of the elements in the group are generators. Thus, we see that the code outputs the two cycles, the identity () and (12).

Parity symmetries

A second interesting type of symmetries is parity symmetries. These symmetries exist in abundance in Hamiltonian systems. In this section, we introduce the relevant background as well as algorithms that generate such symmetries.

Definition 4.2.6. A parity transformation is a map

$$(u_1,..,u_k,x_1,...,x_m) \to Q(z)(u_1,..,u_k,x_1,...,x_m)$$

that flips the sign of z where $z \subset \{u_1, ..., u_k, x_1, ..., x_m\}$.

Proposition 4.2.7. Parity transformations Q(z) acting on $(u_1, ..., u_k, x_1, ..., x_m)$ have two important properties. Let $z = \{a_1, ..., a_n\} \subset \{u_1, ..., u_k, x_1, ..., x_m\}$, where $n \le k + m$. Then,

- $Q(z) = Q(a_1)Q(a_2)...Q(a_n)$.
- The number of all possible parity transformations acting on $(a_1, ..., a_n)$ is 2^n .

Proof. The first statement is obvious from the definition of a parity transformation. The proof for the second statement is as follows. Let $\{a_1, ..., a_n\} \subset \{u_1, ..., u_k, x_1, ..., x_m\}$. For each $a_i \in \{a_1, ..., a_n\}$ we can either flip its sign or leave it unchanged. Hence, the number of parity transformations is 2^n .

Example 4.2.8. Consider a system of PDEs with the variables (u, v, w, t, x, y, z). Then, an example of a parity map,

$$\begin{split} (u,v,w,x,y,z) &\to Q(u,v,y)(u,v,w,x,y,z) = Q(u)Q(v)Q(y)(u,v,w,x,y,z) \\ &= (-u,v,-w,x,-y,z). \end{split}$$

A parity symmetry is defined as follows.

Definition 4.2.9. A parity symmetry is a parity transformation

$$(u_1,...,u_k,x_1,...,x_m) \to Q^s(z)(u_1,...,u_k,x_1,...,x_m)$$

which leaves the system (1.1) unchanged up to a reordering of the equations.

Theorem 4.2.10. Let $z = \{a_1, ..., a_n\} \subset \{u_1, ..., u_k, x_1, ..., x_m\}$. The set of all possible parity transformations Q(z), $G_{parity,z}$, forms a group. Furthermore, the set of all parity symmetries Q^s , $H_{parity,z}$, forms a subgroup of it. That is, $H_{parity,z} < G_{parity,z}$.

Proof. Fix $z = \{a_1, ..., a_n\}$. First, we check if $G_{parity,z}$ obeys the group properties. It is clear from the definition and proposition (4.2.7) that they are closed and associative under the naturally defined operation. Also, the identity element is $Q(\phi)$, where ϕ is the empty set. Finally, the inverse of any element is itself. Thus, $G_{parity,z}$ satisfies the properties of a group.

Second, we check if $H_{parity,z} < G_{parity,z}$. Any parity symmetry is a parity transformation. Thus, $H_{parity,z} \subset G_{parity,z}$. Now, assume that h, f are parity symmetries. Then, hf is a parity symmetry. This follows because each element of $H_{parity,z}$ leaves the system (1.1) unchanged, and so applying the two in a row must also leave it unchanged. Hence, $H_{parity,z}$ is closed under the natural operation. Finally, for any $h \in H_{parity,z}$, $h^{-1} = h \in H_{parity,z}$. Therefore, $H_{parity,z} < G_{parity,z}$.

Remark 4.2.11. We can set z to be either the set of independent or dependent

variables. Thus, the result applies to either of the two separately. In this case, we write $G_{parity,d}$, $H_{parity,d}$ for $z = \{u_1, ..., u_k\}$, and $G_{parity,I}$, $H_{parity,I}$ for $z = \{x_1, ..., x_m\}$. This will prove useful when constructing the next algorithm.

4.2.2 Algorithm II

We introduce a second algorithm that calculates the following:

- The set of collections of independent/dependent symmetries and independent/dependent parity symmetries for a given system of PDEs. We call it Sym.
- The sum $\beta_G(x)$ in (definition 4.1.5) for any quantity.

Remark 4.2.12. Given a system of PDEs, four possible transformations can be performed on its set of variables at once, given by the operators: P_I , P_d , Q_I , Q_d . We notice that these operators don't always commute. For example, $(213)_I(12)_I(u, v, x, y, z) = (u, v, x, z, y) \neq (12)_I(213)_I(u, v, x, y, z) = (u, v, y, z, x)$ However, they always commute when $r_1 \neq r_2$. This suggests that we can consider transformations of independent and dependent variables separately.

Based on the previous remark, one must adopt a convention as to which order the transformations are applied; this is necessary for making sense of the set Sym. Now, we have for each set of variables, independent or dependent, two possible conventions. Then, there are four different possible conventions in total to interpret each element of the set Sym. As we will see, we must have two slightly different versions of the following algorithm.

Let's consider first the following version of the code. We include the other version in appendix B. Here, we assume applying permutations comes before parities.

Before we discuss the details of the code, we have to address the following issue. In theorems 4.2.3 and 4.2.2, we saw that $O_r < S_t$ and $H_{parity,z} < G_{parity,z}$. Now, let's call the set of all collections of independent/dependent transformations and independent

parity transformations Totalset. Given our convention, the set Totalset then is $S_t \times G_{parity,r}$ where $(r,t) \in \{(I,m),(d,k)\}$; and each is a group. It is then necessary to show that the set Sym is a subgroup of Totalset. We introduce next the proof.

Theorem 4.2.13. Sym < Totalset.

Proof. If $s, t \in Sym$, then $st \in Sym$. This is because both of them will leave the system unchanged; applying both in a row then also leaves the system unchanged. Thus, Sym is closed. Next, we show that for any $s \in Sym$, $s^{-1} \in Sym$. Sym is finite, and thus we have $s^k = Id$ for some $k \in \mathbb{N}$. It follows then, by the closure of Sym that $s^{-1} = s^{k-1} \in Sym$. Therefore, Sym is a subgroup of Totalset.

Remark 4.2.14. The result applies for all four possible conventions. It is easy to modify the proof above for each convention by simply accounting for the order of the direct product.

Now, we are ready to introduce our code. First, we set up the data.

```
MKF := Function[#1, #2] &
PDE = {};
DepVarsI = {};
IndVarsI = {};
System2symmetrize = {};
```

PDE is a the list $\{f_1, f_2, ..., f_n\}$ associated with our PDE system (written in the standard form 4.1); System2symmetrize is a list of the quantities to be symmetrized; and MKF is a function that generates functions.

Next, we want to create a function that checks whether a certain element of Totalset is a symmetry; its output, thus, is either True or False. We call this function PDEInv. Here, we represent an element Totalset by the tuple

(PDEPV, PINDV, PADEP, PAIND).

These are permutation transformations of dependent (PDEPV) and independent (PINDV) variables and to parity transformations of dependent (PADEP) and independent (PAIND) variables.

Now, our task is to evaluate this function at all elements of *Totalset*. Note that *PDEInv* is a function of six variables while each element of *Totalset* contains four variables. However, the first two variable, *PPDE* and *extraminus* are introduced to account for a possible reshuffling of an otherwise identical system (after applying the transformation). Hence, it is done for technical reasons and carries no information about the symmetry itself.

To do the evaluations, we use the following code. It produces the set Totalset; then, it produces the set Sym, which is the set of compound symmetries (according

to our convention) for the system:

$$f_1(u_i, x_j, \partial_j u_i) = 0$$

$$f_2(u_i, x_j, \partial_j u_i) = 0$$

$$f_3(u_i, x_j, \partial_j u_i) = 0$$
...
$$f_n(u_i, x_j, \partial_j u_i) = 0.$$

```
where i=1,...,k and j=1,...,m.

Checklist = {PDEInv @@ #, #} & /@

Tuples[{Permutations[Range[Length[PDE]]],

Subsets[Range[Length[PDE]]],

Permutations[Range[Length[DepVarsI]]],

Permutations[Range[Length[IndVarsI]]],

Subsets[Range[Length[DepVarsI]]],

Subsets[Range[Length[IndVarsI]]]];

Collection = Part[#, 2] & /@ Select[Checklist, #[[1]] == True &];

Sym = Part[#, {3, 4, 5, 6}] & /@ Collection
```

Finally, we are interested in finding the sum $\beta_G(x)$ for every element in the list System2symmetrize. The following code generates the list Symmetrized, which is a list of desired sums $\beta_G(x)$.

```
ggg[PPDE_, extraminus_, PDEPV_, PINDV_, PADEP_, PAIND_] :=
Module[{p0, p2, p3, p4, g, jj},
   g[p0_] := 1;
   g[p0_] := -1 /;
   MemberQ[ Map[List, PADEP], Flatten[Position[DepVarsI, p0]]];
```

Symmetrized = 1/Length[Sym] * Total[ggg @@ # & /@ Sym, 1]

4.2.3 An illustration

We illustrate the usage of the previous code with the following examples:

Example 4.2.15. We want to use the code to generate all permutation and parity symmetries for the following PDE system, given that we apply parity transformations first.

$$\begin{cases} u_t = x^3 y v u_x^2 \\ v_t = x y^3 u v_y^2. \end{cases}$$

$$(4.4)$$

Also, we want to symmetrize the following set of quantities under the generated group of symmetries, Sym.

$$\{u^2u_x^2, v^2v_x^2, u^2v, u, v\}.$$

We set up the data as follows:

MKF := Function[#1, #2] &

PDE = $\{x^3 \ y \ v[x, y] \ D[u[x, y], \{x, 1\}]^2,$ $x \ y^3 \ u[x, y] \ D[v[x, y], \{y, 1\}]^2\};$

DepVarsI = {u, v};

IndVarsI = $\{x, y\}$;

System2symmetrize = $\{u[x, y]^2 D[u[x, y], \{x, 1\}]^2,$

 $v[x, y]^2 D[v[x, y], \{x, 1\}]^2, u[x, y]^2 v[x, y], u[x, y], v[x, y];$

We then run the rest of the code. We get the following set Sym:

{{{1, 2}, {1, 2}, {}, {}}, {{1, 2}, {1, 2}, {1, 2}}, {{1,

- 2}, {1, 2}, {1}}, {{1, 2}, {1,
- 2}, {1}, {1}}, {{1, 2}, {1, 2}, {1}, {2}}, {{1, 2}, {1,
- 2}, {2}, {}}, {{1, 2}, {1, 2}, {1, 2}}, {{1, 2}
- 2}, {1}, {}}, {{1, 2}, {1, 2}, {1, 2}}, {{1, 2}
- 2}, {2}, {1}}, {{1, 2}, {1, 2}, {2}}, {{1, 2}, {1,
- 2}, {}, {1}}, {{1, 2}, {1, 2}, {2}}, {{1, 2}, {1, 2}, {1,
- 2}, {}}, {{1, 2}, {1, 2}, {1, 2}}, {{2, 1}, {2,
- 1}, {}, {}}, {{2, 1}, {2, 1}, {1, 2}}, {{2, 1}, {1,
- 2}, {1}}, {{2, 1}, {2, 1}, {1, 2}, {2}}, {{2, 1}, {2,
- 1}, {1}, {1}}, {{2, 1}, {2, 1}, {2}}, {{2, 1}, {2,
- 1}, {2}, {}}, {{2, 1}, {2, 1}, {2}, {1, 2}}, {{2, 1}, {2,
- 1}, {1}, {}}, {{2, 1}, {2, 1}, {1, 2}}, {{2, 1}, {2,
- 1}, {2}, {1}}, {{2, 1}, {2, 1}, {2}}, {{2, 1}, {2,
- 1}, {}, {1}}, {{2, 1}, {2, 1}, {2}}, {{2, 1}, {1,
- 2}, {}}, {{2, 1}, {2, 1}, {1, 2}, {1, 2}}}

Sym is a list of sublists, each representing a symmetry. Each symmetry, in turn, is a list of four sublists itself; to show how these four sublists are to be interpreted, we examine the following symmetry.

{{1, 2}, {1, 2}, {1, 2}, {1}}

The first two elements $\{1,2\}$, $\{1,2\}$ are permutations of the dependent and independent variables, respectively. A permutation of n variables in general is written as $\{P(1), P(2), ..., P(i), ..., P(n)\}$, where $1 \leq P(i) \leq n$ represents the new position of the ith element. Thus, in our example, all of these permutations represent identity permutations.

The last two elements $\{1,2\}$, $\{1\}$ represent parity transformations of the dependent and independent variables, respectively. Here, they represent multiplying the first and second elements of DepVarsI as well as the first element of IndVarsI, namely the variables $\{u, v, x\}$, by -1.

Remark 4.2.16. Note that the previous set Sym is not for the system (4.4). It is, rather for the system

$$\begin{cases} x^3 y v u_x^2 = 0 \\ x y^3 u v_y^2 = 0. \end{cases}$$

The set Sym for (4.4) is a subset of the one above. Specifically, it is the subset that leave the dependent variables, $\{u, v\}$, invariant. Our code doesn't attempt to find such a subset directly. This is because we want it to work for any general set of polynomials. However, one can easily find the subset by generating a different set Sym for the system $PDE = \{u[x, y], v[x, y]\}$; and then by finding the intersection of the two Sym sets.

Next, we run the last part of the code to symmetrize each quantity in the list under the set Sym. In other words, we generate the set Symmetrized for

$$\{u^2u_x^2, v^2v_x^2, u^2v, u, v\}$$

The output is as follows:

Thus, the symmetrization of $u^2u_x^2$ and $v^2v_x^2$ is the same, namely, $\frac{1}{2}[u^2u_x^2 + v^2v_x^2]$; and the symmetrization for the other elements is 0. The interesting part here is that we found that two different elements of our list are the same under the action of a group of discrete symmetries.

Example 4.2.17. Let's consider the Hirota-Satsuma system of PDEs used in the study of shallow water waves.

$$u_{t} = \frac{1}{2}u_{xxx} + 3uu_{x} - 6vv_{x},$$

$$v_{t} = -v_{xxx} - 3uv_{x}.$$
(4.5)

We also want to symmetrize the following list:

$$\{u^2u_r^2, uv, u, v\}$$

The set-up part of the code looks like:

```
MKF := Function[#1, #2] &
PDE = {1/2 D[u[x], {x, 3}] + 3 u[x] D[u[x], {x, 1}] -
        6 v[x] D[v[x], {x, 1}], -D[v[x], {x, 3}] - 3 u[x] D[v[x], {x, 1}]};
DepVarsI = {u, v};
IndVarsI = {x};
System2symmetrize = {u[x]^2 D[u[x], {x, 1}]^2, v[x] u[x], v[x],
        u[x] };
```

Then, we run the code to get the following set Sym:

Furthermore, the set Symmetrized for $\{u^2u_x^2, uv, u, v\}$ is:

$$\{u[x]^2 D[u[x],\{x,1\}]^2, 0, u[x], 0\}$$

Remark 4.2.18. Here, an interesting result is that both $u^2u_x^2$ and u are fixed under the action of the group.

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APPENDICES

A Appendix I

A.1 Differentiable Manifolds

Here, we introduce the concept of a smooth manifold. We start with the definition of an atlas.

Definition A.1.1. Let U be a subset of an abstract set M. A coordinate chart is one-to-one mapping $\gamma \colon U \to \mathbb{R}^n$ such that $\gamma(U)$ is an open subset of \mathbb{R}^n

Remark A.1.2. The set U is called a coordinate patch. The components of $\gamma(U)$ are called local coordinates. Finally, the inverse mapping $\gamma^{-1}(U)$ is called parametrization.

Definition A.1.3. Two coordinate charts $\gamma_1: U_1 \to \mathbb{R}^n$ and $\gamma_2: U_2 \to \mathbb{R}^n$ are mutually compatible if the map $\gamma_2 \circ \gamma_1^{-1}$, whose domain is $\gamma_1(U_1 \cap U_2)$, is a diffeomorphism with a smooth inverse. These mapping are called transition maps (or change-of-coordinates transformations)

Definition A.1.4. An n-dimensional atlas for a set M is a family of mutually compatible n-dimensional coordinate charts covering M. Two atlases are equivalent if all of their charts are mutually compatible; we call this equivalence relation R.

Now, we are ready to define differential structures on manifolds.

Definition A.1.5. A smooth structure (or differential structure) is an equivalence class of atlases for M modulo R. Any atlas in this class is said to determine the smooth structure.

Finally, we introduce the definition of a smooth manifold.

Definition A.1.6. A smooth manifold is a set M with a smooth structure.

A.2 Tensors

There are two types of tensors: covariant and contravariant. We define both types as follows:

Definition A.2.1. A covariant k-tensor on a finite-dimensional, real vector space V is a multilinear mapping

$$T:V\times\ldots\times V\to\mathbb{R}$$

where V being multiplied k times.

Similarly,

Definition A.2.2. A contravariant k-tensor on a finite-dimensional, real vector space V is a multilinear mapping

$$T: V^* \times ... \times V^* \to \mathbb{R}$$

where V^* is the dual space of V. It is also being multiplied k times.

Remark A.2.3. We can extend the domain of tensors from linear spaces to any manifold Q. We do this by defining tensors on the tangent space based at a point q, T_qQ . For example, a covariant k-tensor on the tangent space of T_qQ a configuration space Q is the mapping:

$$T: T_qQ \times ... \times T_qQ \to \mathbb{R}$$

where V being multiplied k times.

Definition A.2.4. A covariant tensor field on a manifold M is a family of smoothly varying rank-k tensors [T(z)]. Here, T(z) is defined on the tangent space T_zM

Definition A.2.5. (Differential n-forms) A differential n-form is a skew-symmetric covariant tensor field of rank n.

Now, we are ready to introduce differential 1-forms and vector fields.

Definition A.2.6. (Differential 1-forms) A differential 1-form on a manifold M is a map

$$\theta: M \to T^*M$$

such that $\theta(z) \in T_z^*M$, the cotangent space at z, for any $z \in M$

Properties:

- $(\theta_1 + \theta_2)(z) = \theta_1(z) + \theta_2(z)$
- $(k\theta)(z) = k(z)\theta(z)$ where $k: M \to \mathbb{R}$ (a scalar field)

Definition A.2.7. (Vector fields) A vector field on a manifold M is a map

$$X: M \to TM$$

such that $X(z) \in T_zM$, the tangent space at z, for any $z \in M$

Properties:

- $(X_1 + X_2)(z) = X_1(z) + X_2(z)$
- (kX)(z) = k(z)X(z) where $k: M \to \mathbb{R}$ (a scalar field)

B Appendix II

B.1 Mathematica code

In this appendix, we include the second version of our code.

The first function

```
PDEInv[PPDE_, extraminus_, PDEPV_, PINDV_, PADEP_, PAIND_] :=
Module[{p0, p1, p2, p3, p4, g, jj}, g[p0_] := 1;
g[p0_] := -1 /;
    MemberQ[Map[List, PADEP], Flatten[Position[DepVarsI, p0]]];
p4 = Permute[MapAt[Minus, IndVarsI, Map[List, PAIND]], PINDV];
p3 = MKF[Permute[IndVarsI, PINDV],
    g[#] # @@ Permute[MapAt[Minus, IndVarsI, Map[List, PAIND]],
        PINDV]] & /@ Permute[DepVarsI, PDEPV];
p2 = MKF[Join[DepVarsI , IndVarsI], PDE] @@ Join[p3, p4];
p1 = Permute[p2, PPDE];
jj = MKF[Permute[IndVarsI, PINDV], # @@ IndVarsI] & /@ DepVarsI;
MapAt[Minus, MKF[DepVarsI, p1] @@ jj, Map[List, extraminus]] ===
    PDE
]
```

The second function

```
ggg[PPDE_, extraminus_, PDEPV_, PINDV_, PADEP_, PAIND_] :=
```

```
Module[{p0, p2, p3, p4, g, jj},
  g[p0_] := 1;
  g[p0_] := -1 /;
    MemberQ[ Map[List, PADEP], Flatten[Position[DepVarsI, p0]]];
  p4 = Permute[MapAt[Minus, IndVarsI, Map[List, PAIND]], PINDV];
  p3 = MKF[Permute[IndVarsI, PINDV],
        g[#] # @@ Permute[MapAt[Minus, IndVarsI, Map[List, PAIND]],
        PINDV]] & /@ Permute[DepVarsI, PDEPV];
  p2 = MKF[Join[DepVarsI , IndVarsI], PDE] @@ Join[p3, p4];
  jj = MKF[Permute[IndVarsI, PINDV], # @@ IndVarsI] & /@ DepVarsI;
  MKF[DepVarsI, p2] @@ jj
]
```