Theory and Construction of Structure Preserving Integrators in Poisson Geometry

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Thèse

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RÉSUMÉ

Mots-clefs: Intégrateurs géométriques, systèmes hamiltoniens, géométrie de Poisson, systèmes dynamiques, groupoïde symplectique

Cette thèse est motivée par des applications en analyse numérique et porte sur la géométrie de Poisson et la géométrie de Dirac.

Nous résumons ici les principaux résultats de la thèse.

- Nous introduisons pour toute structure de Poisson π sur une variété M la notion de bi-réalisation, et l'illustrons par l'exemple sur les crochets de Poisson constants, linéaires, et certains crochets quadratiques. Dans cette bi-réalisation, nous démontrons que le flot hamiltonien d'un hamiltonien quelconque H se reformule par une équation aux dérivées partielles de Hamilton-Jacobi en transformant H en une famille $\mathcal{C}^\infty$ de fonctions sur M dépendantes du temps $S(H) = S_t(H)$ dont l'existence est assurée localement pour des petites valeurs de t.

- Nous définissons les intégrateurs de Poisson hamiltoniens comme des intégrateurs de Poisson dont la trajectoire discrète suit le flot d'un hamiltonien dépendant du temps et expliquons, par l'exemple d'abord, en quoi ils sont une généralisation naturelle des intégrateurs symplectiques pour une structure de Poisson quelconque. Par la suite, une construction générale d'un intégrateur de Poisson hamiltonien pour une structure de Poisson π, un hamiltonien H, un ordre k et un pas de temps Δt quelconques sont donnés via la troncature à l'ordre k de la transformée de Hamilton-Jacobi $S_{\Delta t}(H)$ du hamiltonien H sur une bi-réalisation de la structure de Poisson π. Nous définissons également la suite de Farmer et expliquons comment elle fournit des formules récursives explicites pour résoudre l'équation de Hamilton-Jacobi à un ordre arbitraire.

- Pour une famille $\mathcal{C}^\infty$ de sous-variétés lagrangiennes $\mathscr{L}$ d'une variété symplectique, nous construisons une famille de 1-formes fermées appelée 1-forme de variation de $\mathscr{L}$ et démontrons par suite une correspondance canonique, dans un groupoïde symplectique local, entre les familles de bi-sections lagrangiennes et les doublets formés d'une bi-section lagrangienne et d'une famille $\mathcal{C}^\infty$ de 1-formes fermées sur la base. Nous expliquons comment cela founrit une interprétation géométrique des intégrateurs de Poisson hamiltoniens à travers la notion de bi-réalisation.

- Nous définisssons pour tout hamiltonien dépendant du temps $(H_t)_{t\in I} \in \mathcal{C}^\infty(I \times M)$ une série formelle $\mathcal{M}_\epsilon(H) \in \mathcal{C}^\infty(M)\,[[\epsilon]]$, dite série de Magnus, dont on démontre que le flot hamiltonien au temps 1 est formellement égal au flot de $(H_t)_{t\in I}$ au temps ϵ. En l'appliquant aux hamiltoniens dépendants du temps correspondants aux intégrateurs de Poisson précédemment construits, nous démontrons l'existence pour ces méthodes numériques d'un hamiltonien modifié.

- Finalement, nous comparons nos méthodes numériques avec les méthodes de Runge-Kutta sur l'exemple du solide rigide et des équations de Lotka-Volterra. À l'inverse de ceux existants, nous observons pour nos algorithmes la préservation des Casimirs à la précision machine et l'oscillation des trajectoires discrètes autour du niveau du hamiltonien, oscillation dont l'amplitude est contrôlée par l'ordre de la méthode. Nos intégrateurs de Poisson hamiltoniens sont aussi testés sur un système de Lotka-Volterra dont la trajectoire part à l'infini et l'on démontre numériquement, comparés aux méthodes Runge-Kutta, un meilleur comportement au voisinage de cette singularité, bien que l'ordre de notre méthode soit sur cet exemple choisi moins élevé.

En appendice, nous rappelons quelques élements de théorie des groupoïdes symplectiques locaux préliminaires à la construction d'intégrateurs hamiltoniens de Poisson.

Nous résumons ici les résultats de géométrie de Dirac.

- Nous introduisons la cohomologie horizontale $\mathcal{H}^\bullet_{hor}$ d'une algébroïde et, dans le cas particulier d'une structure de Dirac $D \to M$, étudions son 2-cocycle canonique ω_D et son annulation en cohomologie sur les exemples classiques des feuilletages réguliers, des structures présymplectiques et des structures de Poisson.
- Sous condition suffisante de l'exactitude de $[\omega_D]$ dans $\mathcal{H}^2_{hor}(D)$ et pour tout hamiltonien $H \in \mathcal{C}^\infty(M)$, nous exhibons une fonctionnelle dont les points critiques sont exactement les courbes intégrales des champs de vecteurs hamiltoniens de H, c'est-à-dire les sections $X \in \mathfrak{X}(M)$ tels que $(X, \mathrm{d}H) \in \Gamma(D)$.
- Toujours sous couvert de la nullité de $[\omega_D]$, nous déduisons du précédent résultat une généralisation de la transformée de Legendre aux structures de Dirac.

ABSTRACT

Keywords: Geometric integrators, Hamiltonian systems, Poisson geometry, dynamical systems, symplectic groupoids

This thesis is motivated by applications in numerical analysis and deals with Poisson and Dirac geometry.

We sum up here the main results of this thesis.

- We introduce for any Poisson structure π on a manifold M the notion of bi-realisation and illustrate it by examples on constant, linear and some quadratic Poisson brackets. In that bi-realisation, we show that the Hamiltonian flow of a Hamiltonian H can be reformulated through Hamilton-Jacobi equation by transforming H into a smooth family of time-dependent functions on M $S(H) = S_t(H)$, for which existence is ensured for small values of t.

- We define Hamiltonian Poisson integrators as Poisson integrators for which discrete trajectory follows the flow of a time-dependent Hamiltonian and we explain, by an example at first, how they are a natural generalisation of symplectic integrators for a generic Poisson structure. Next, a construction of a Hamiltonian Poisson integrator for generics Poisson structure π, Hamiltonian H, order k and time-step Δt are given via any truncation at order k of the Hamilton-Jacobi transform $S_{\Delta t}(H)$ of the Hamiltonian H on a bi-realisation of the Poisson structure π. We also define the Farmer sequence and we explain how it gives explicit recursive formulae to solve Hamilton-Jacobi equation at an arbitrary order.

- For a smooth family of Lagrangian submanifolds $\mathscr{L}$ of a symplectic manifold, we construct a family of closed 1-forms named variation form of $\mathscr{L}$ and we show a canonical correspondence, in a local symplectic groupoid, between families of Lagragnian bi-sections and couples made of a Lagrangian bi-section and a smooth family of closed 1-forms on the base. We explain how this gives a geometric interpretation of Hamiltonian Poisson integrators through the notion of bi-realisation.

- We define for any time-dependent Hamiltonian $(H_t)_{t\in I} \in \mathcal{C}^\infty(I \times M)$ a formal series $\mathcal{M}_\epsilon(H) \in \mathcal{C}^\infty(M)\,[[\epsilon]]$ named Magnus series, for which we show that its time 1 Hamiltonian flow is formally equal to the Hamiltonian flow of $(H_t)_{t\in I}$ at time ϵ. By applying it to time-dependent Hamiltonians corresponding to the previously constructed Hamiltonian Poisson integrators, we show the existence for those numerical methods of a modified Hamiltonian.

- To conclude, we compare our integrators with Runge-Kutta methods on the example of rigid body dynamics and Lotka-Volterra differential equations. Unlike existing methods, we observe for our algorithms Casimir preservation at required precision and oscillation of discrete trajectories around a level of the Hamiltonian, the amplitude of those oscillations being controlled by the order of the method. Our Hamiltonian Poisson integrators are also benchmarked on a Lotka-Volterra system for which the trajectory diverges to infinity. We show through numerical simulations a better behaviour in a neighborhood of this singularity compared to Runge-Kutta methods, even if the order of our method is chosen to be lower.

We recall in appendix some theory of local symplectic groupoids that is preliminary to our construction of Hamiltonian Poisson integrators.

We sum up here Dirac geometry results.

- We introduce the horizontal cohomology $\mathcal{H}^\bullet_{hor}$ of a Lie algebroid and, in the particular case of a Dirac structure $D \to M$, we study its canonical 2-cocycle ω_D and its vanishing in cohomology on classical examples such as regular foliations, pre-symplectic structures and Poisson structures.
- Under the sufficiency condition of the exactness of $[\omega_D]$ in $\mathcal{H}^2_{hor}(D)$ and for any Hamiltonian $H \in \mathcal{C}^\infty(M)$, we exhibit a functional for which critical points are exactly integral curves of Hamiltonian vector fields of H, i. e. sections $X \in \mathfrak{X}(M)$ such that $(X, \mathrm{d}H) \in \Gamma(D)$.
- Under the same vanishing assumption of $[\omega_D]$, we deduce from the previous result a generalisation of the Legendre transform to Dirac structures.

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Contents

CHAPTER 1

A motivation for new geometric integrators

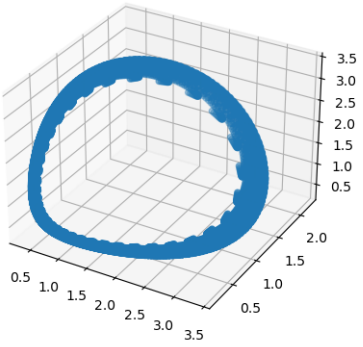


Figure 1.1: Long run simulation of the Runge-Kutta 2 method for a periodic orbit of equation (1.2)

The system of differential equations

$$\dot{x}_j = \epsilon_j x_j + \sum_{k=1}^{n} a_{jk} x_j x_k, \ j \in [\![1, n]\!] \tag{1.1}$$

was used by Vito Volterra in his *Leçons Mathématiques sur la Lutte pour la Vie* [72] as a model in population dynamics. $(x_j)_j$ stands for the collection of species populations and $(\epsilon_j)_j$ and $(a_{jk})_{jk}$ are real parameters describing respectively inner properties and interactions of species. The general behaviour of (1.1) is intricate and has been extensively studied from a qualitative aspect (see [57, 21, 41] to cite a few). The rich dynamics of (1.1) emphasizes not only the fact that integrating by quadratures a generic differential equation is hopeless, but also how it requires robust numerical tools to study it. Indeed, we illustrate on a very simple 3-dimensional particular case of Volterra's equation the advantages of numerical methods constructed on geometric features of the dynamical system.

Let us set $n = 3$, $\epsilon = \begin{pmatrix} 2 \\ 0 \\ -2 \end{pmatrix}$ and $a = \begin{pmatrix} 0 & 1 & 1 \\ -1 & 0 & 1 \\ -1 & -1 & 0 \end{pmatrix}$. The system becomes

$$\begin{cases} \dot{x} &= x(y+z) - 2x \\ \dot{y} &= y(z-x) \\ \dot{z} &= -z(x+y) + 2z \end{cases} . \tag{1.2}$$

Setting $x_0 = \begin{pmatrix} 2 \\ 2 \\ 2 \end{pmatrix}$, it can be shown that the trajectory $x(t)$ exists for all t and is periodic. However, a traditional method fails to preserve the periodicity of the computed trajectory by destroying its topology itself: the Runge-Kutta method with time-step $\Delta t = 10^{-1}$ gives a discrete trajectory that even runs to infinity as the amount of iteration grows. The 10^4 first iterations are plotted figure 1.1.

Such numerical issues have been noticed by engineers in the mid twentieth century ([71]) and have motivated the development of *geometric integrators*, i.e. numerical methods for which the construction relies on geometric structures of the equation we solve numerically. Those methods typically proved to perform better on long run simulations, remedying problems such as the one occuring in figure (1.1). The first ones to be developped were so-called *symplectic integrators* and designed for Hamiltonian systems in the context of symplectic geometry, meaning that the differential equation is of the form

$$\begin{pmatrix} \dot{q} \\ \dot{p} \end{pmatrix} = J \cdot \nabla H(q,p) = \begin{pmatrix} -\partial_p H \\ \partial_q H \end{pmatrix} . \tag{1.3}$$

Such integrators have been extensively studied both from theoretical ([32, 5]) and practical aspects. Their stability has found successful applications in various fields such as molecular dynamics ([70]) or cosmology ([20]). In the latter, a simulation of the universe is performed to understand patterns in long term accretion of galaxies, achieving long run numerical simulations of the N-body problem for N about 11 000.

However, such symplectic integrators are of no help for equation (1.1) since the equation is not of the form (1.3). Instead of being Hamiltonian for the symplectic structure J, Volterra's equations are Hamiltonian for a *Poisson structure*, meaning that J is replaced by a matrix $\pi(x)$ that is still skew-symmetric but with its rank dropping from one point to another:

$$\dot{x} = \pi(x) \cdot \nabla H(x). \tag{1.4}$$

Equation (1.2) is Poisson Hamiltonian for $\pi(x) = \begin{pmatrix} 0 & x_1x_2 & x_1x_3 \\ -x_1x_2 & 0 & x_2x_3 \\ -x_1x_3 & -x_2x_3 & 0 \end{pmatrix}$ and $H(x) = \sum_{i=1}^{3} x_i - \log(x_i)$.

Generic Hamiltonian systems for a Poisson structure differ greatly from (1.3) in terms of symmetries and singularities. Their genericity allows a wider class of the latter ones. In turn, Poisson Hamiltonian systems appear in many classes of dynamical systems coming from conservative mechanics ([47, 1]), often related to reduction theory. Furthermore, symplectic integrators cannot be applied on a general equation of the form (1.4), hence the need of a notion of *Poisson integrator*.

Still, first attempts of Poisson integrators were based on straightforward generalisation of symplectic integrators using local normal forms of Poisson structure. Darboux-Weinstein theorem ([18]) states that any Poisson structure $\pi(x)$ is locally of the form $\begin{pmatrix} J & 0 \\ 0 & 0 \end{pmatrix}$, transforming (1.4) into

$$\begin{pmatrix} \dot{q} \\ \dot{p} \\ \dot{c} \end{pmatrix} = \begin{pmatrix} -\partial_p H(q,p,c) \\ \partial_q H(q,p,c) \\ 0 \end{pmatrix}. \tag{1.5}$$

There, symplectic integration may apply by ignoring the c variable. However, this approach faces two main drawbacks :

- although it can be achieved in particular cases ([38]), finding the transformation that takes a generic $\pi(x)$ to $\begin{pmatrix} J & 0 \\ 0 & 0 \end{pmatrix}$ is in general as hard as solving (1.4),
- this approach requires an individual treatment of each singularity, since Darboux transformation around a point x_0 depends on the behaviour of $\pi(x)$ around x_0, for instance on variations of the rank of π.

Another approach is based on splittings and gave successful results in particular cases ([56]) – even generating interesting related algebraic theory ([39]) – although it is based on explicit integration and therefore cannot be claimed as an anolog of symplectic integrators for Poisson Hamiltonian systems. (1.1) is already a motivation for the search of Poisson integrators for a generic Hamiltonian, since physically relevant parameters occur in the system and pop up in the Hamiltonian itself[1].

A modern approach to Poisson integrators is geometric and related to the integration of the Lie bracket $\{.,.\}$ associated to π. Roughly speaking, two operations can be done to the Poisson structure π :

- **symplectic realization:** replacing π by J, i.e. *killing singularities* of π, by doubling dimension ([22]),
- **higher integration:** integrating the Lie bracket $\{.,.\}$ to a group[2] the same way a Lie algebra integrates to a Lie group, this very wide group allowing, in turn, to recover *symmetries* of the space we started with. This large group admits a finite-dimensional structure if one replaces its product by a local groupoid multiplication law, a notion that is out of the reach of this introduction. We come back to it later.

The object we obtain by combining those two items is related to the notion of *local symplectic groupoid*. Several attempts have been made to use it for the task of numerical integration of Poisson Hamiltonian systems (see [26, 27, 37] and [23] for an inspiring particular case).

The aim of this thesis is to carry out this local symplectic groupoid approach of numerical integration for a general Poisson Hamiltonian system of the form (1.4) and to perform a theoretical study of resulting discrete trajectories.

Since we think it encapsulates the spirit of the thesis, we say a few words on the way local symplectic groupoids appear in our construction of numerical methods. We use it by introducing the notion of *bi-realisation*, which is a coordinate version of the former. The Poisson integrators we construct are built using the k-th jet of the exact geometric object on the bi-realisation corresponding to the dynamics we discretize. The study of the geometry of the local symplectic groupoid gives geometric properties of the numerical methods and coordinates for the bi-realisation allow to use it for

[1] although not every equation of the form (1.1) is Poisson Hamiltonian, see [21] for details

[2] Rybicki studied rigorously in [61] the question of integration of Poisson algebras to infinite dimensional Lie groups.

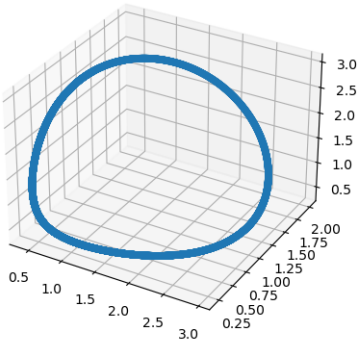


Figure 1.2: Hamiltonian Poisson method at order 1 for equation (1.2)

numerical computations. For equation (1.2) at order 1 and with time-step Δt, our obtained numerical scheme is unexpected:

1. starting from $\begin{pmatrix} x_n \\ y_n \\ z_n \end{pmatrix}$, solve the non-linear equation in $\begin{pmatrix} \tilde{x}_n \\ \tilde{y}_n \\ \tilde{z}_n \end{pmatrix}$,

$$\begin{cases} e^{(\frac{-\Delta t}{2}(\tilde{y}_n+\tilde{z}_n-2))}\tilde{x}_n & = x_n \\ e^{(\frac{\Delta t}{2}(\tilde{x}_n-\tilde{z}_n))}\tilde{y}_n & = y_n \\ e^{(\frac{\Delta t}{2}(\tilde{x}_n+\tilde{y}_n+2))}\tilde{z}_n & = z_n \end{cases}$$

2. and set

$$\begin{cases} x_{n+1} & = e^{(\frac{\Delta t}{2}(\tilde{y}_n+\tilde{z}_n-2))}\tilde{x}_n \\ y_{n+1} & = e^{(\frac{\Delta t}{2}(-\tilde{x}_n+\tilde{z}_n))}\tilde{y}_n \\ z_{n+1} & = e^{(\frac{-\Delta t}{2}(\tilde{x}_n+\tilde{y}_n+2))}\tilde{z}_n \end{cases} .$$

We show on figure 1.2 the simulation of equation (1.2) with our above described methods, where we set same parameters as for 1.1. The integrator we use here is of order 1. The result of the numerical simulation is a discrete trajectory oscillating around the periodic one at an amplitude controlled by the order of the method in a sense we detail in section 4.2.

More generally, the obtained Hamiltonian Poisson integrators have remarkable qualitative properties, for instance in terms of preservation of symmetries or stability around a singularity. Moreover, their geometric construction allows a fine theoretical study of their behaviour.

The thesis is organized as follows.

Chapter 2 is devoted to a summary and a simplified presentation of the main results of the thesis. We introduce there the notion of bi-realisation of a Poisson structure and explain how it allows to construct Hamiltonian Poisson integrators through Hamilton-Jacobi equation. A theoretical study of the latter is carried out, as well as a theoretical study of the obtained numerical methods.

Chapter 3 contains the geometric approach to the question of Poisson integrators. The main object underlying their construction is the local symplectic groupoid. Therefore, this chapter collects proofs and results expressed in terms of symplectic groupoids. We also prove here theorems of chapter 2, in particular the ones about truncated solutions of Hamilton-Jacobi equation and analysis of discrete trajectories of Hamiltonian Poisson integrators.

In chapter 4, we implement and benchmark various Poisson integrators to illutrate benefits of the notion of Hamiltonian Poisson integrators. Our numerical simulations confirm theoretical results of the previous chapters.

Chapter 5 is an on-going parallel project about the search of a construction of integrators preserving a Dirac structure. We present results that reformulate Dirac Hamiltonian dynamics in a variational principle under a cohomological assumption.

To conclude, chapter 6 gathers perspectives concerning our variational principle for dynamics on Dirac structures on one side, and our Hamiltonian Poisson integrators on the other side.

CHAPTER 2

Summarized results for Poisson integrators

2.1 Geometric integrators for Poisson Hamiltonian systems

2.1.1 Poisson structures: definition

Let us briefly recall[1] what are Poisson bivector fields and Hamiltonian differential equations, and why they matter. In mechanics, quite some differential equations governing a motion $x(t)$ valued in an open subset $\mathcal{U} \subset \mathbb{R}^n$ take the form:

$$\left\{ \begin{array}{rcl} \dot{x}_1(t) & = & \sum_{j=1}^{n} \pi_{1j}(x(t)) \, \dfrac{\partial H(x(t))}{\partial x_j} \\ & \vdots & \\ \dot{x}_n(t) & = & \sum_{j=1}^{n} \pi_{nj}(x(t)) \, \dfrac{\partial H(x(t))}{\partial x_j} \end{array} \right. \tag{2.1}$$

where $H : \mathcal{U} \longrightarrow \mathbb{R}$ is a smooth function, that it is customary to call *Hamiltonian* in this context, and (π_{ij}), $i, j \in \{1, \ldots, n\}$ is a family of smooth functions which satisfy

$$\pi_{ji} = -\pi_{ij} \quad \text{and} \quad \sum_{a=1}^{n} \frac{\partial \pi_{ij}}{\partial x_a} \, \pi_{ak} + \circlearrowleft = 0, \tag{2.2}$$

where all indices $i, j, k \in \{1, \ldots, n\}$ and $\circlearrowleft$ stands for their cyclic permutations.

Let us first explain these conditions: there is a theorem (see chapter 1 of [43]) claiming that a family $(\pi_{ij}), i, j \in \{1, \ldots, n\}$ of smooth functions on $\mathcal{U} \subset \mathbb{R}^n$ satisfies (2.2) if and only if the bilinear map:

$$\begin{array}{rccl} \{\cdot, \cdot\} : & \mathcal{C}^\infty(U) \times \mathcal{C}^\infty(U) & \longrightarrow & \mathcal{C}^\infty(U) \\ & f, g & \mapsto & \sum_{i,j=1}^{n} \frac{1}{2} \pi_{ij}(x) \left(\dfrac{\partial f}{\partial x_i} \dfrac{\partial g}{\partial x_j} - \dfrac{\partial g}{\partial x_i} \dfrac{\partial f}{\partial x_j} \right) \end{array} \tag{2.3}$$

is a Lie bracket, i.e. is anti-symmetric and satisfies the Jacobi identity:

$$\{f, g\} = -\{g, f\} \text{ and } \{\{f, g\}, h\} + \{\{g, h\}, f\} + \{\{h, f\}, g\} = 0 \tag{2.4}$$

[1] A reader familiar with Poisson geometry may safely skip this section up to 2.1.3.

for all $f, g, h \in \mathcal{C}^\infty(M)$.

Equivalently, the functions $\pi_{ij}(x)$ above can be considered as being a *tensor*, i.e. a map from $\mathcal{U} \subset \mathbb{R}^n$ to $so(n, \mathbb{R})$, viewed as a $n \times n$ matrix depending on x:

$$\begin{array}{rccc} \pi: & \mathcal{U} & \longrightarrow & so(n,\mathbb{R}) \\ & x & \mapsto & (\pi_{ij}(x)_{i,j=1}^n) \end{array},$$

such that the associated bracket (2.3) verifies Jabobi relation (2.4). This is the way we define Poisson structures below.

Definition 2.1.1. A *Poisson structure* on an open subset $\mathcal{U} \subset \mathbb{R}^n$ is a tensor π on $\mathcal{U}$ such that the bilinear map $\mathcal{C}^\infty(\mathcal{U}) \times \mathcal{C}^\infty(\mathcal{U}) \to \mathcal{C}^\infty(\mathcal{U})$ defined by

$$\{f, g\}(x) = {}^t\nabla_x f.\pi(x).\nabla_x g$$

satisfies the skew-symmetry and Jacobi identities (2.4). Equivalently, Poisson structures can be seen as tensors whose coefficients $(\pi_{ij}(x)), i, j \in \{1, \ldots, n\}$ satisfy[2] equations (2.2).

The long history behind this notion comes with a vocabulary, which is sometimes confusing: it is customary to call the bilinear map $\{\cdot, \cdot\}$ the *Poisson bracket*. Also, functions in $\mathcal{C}^\infty(\mathcal{U})$ are – depending on the context – sometimes all called *Hamiltonian functions* or simply *Hamiltonians*. Last, using property of the derivation with respect to the product of functions, the easy to check relation:

$$\{f, gh\} = \{f, g\}h + g\{f, h\}$$

is called *Leibniz identity*. For examples of Poisson structures that appear in mechanics, see section 2.2.3.

We saw that a Poisson structure associates to *two* smooth functions $f, g \in \mathcal{C}^\infty(U)$ another smooth function $\{f, g\}$. But it also allows to associate to *one* Hamiltonian function $H \in \mathcal{C}^\infty(U)$ a first order autonomous differential equation, as in (2.5). More abstractly, (2.5) means that to a Hamiltonian function H we associate the (vector) differential equation:

$$\dot{x}(t) = \pi(x(t)) \cdot \nabla_{x(t)} H. \tag{2.5}$$

We say that a first order autonomous differential equation of the form (2.5) above is a *Hamiltonian differential equation for* (π, H). The reader may note that if $H = H_t$ depends on time, the equation becomes non-autonomous. We will use this extension of the notion later on.

Remark 2.1.2. In differential geometry, a first order differential equation on an open subset U of $\mathbb{R}^n$ with an independent parameter having the meaning of time

$$\dot{x} = F(x) \tag{2.6}$$

is generally referred to as a vector field on U. Moreover, rather than considering only open subsets of $\mathbb{R}^n$, the phase space is often assumed to be a differential manifold.

[2]The Schouten bracket $[.,.]_S$ on tensors, see for instance [22], allows to rephrase the Jacobi condition (2.4) for the tensor π into $[\pi, \pi]$.

2.1.2 The underlying geometry of a Poisson structure

It is natural to ask why it matters that behind an autonomous first order differential equation, there is a Poisson structure and a Hamiltonian function. What does one gain by knowing that a given differential equation is Hamiltonian of (π, H)? The classical answer is that many "quantities" related to π or H are preserved under the flow of the differential equation.

More precisely, any solution $x(t)$ (i. e. an integral curve) of a Hamiltonian differential equation for (π, H) has the following properties:

1. H is a constant of motion, i.e. $H(x(t)) = H(x(0))$. In words, it means that the flow of a Hamiltonian differential equation for (π, H) preserves the level sets of the Hamiltonian function H.

2. More generally, any function G such that $\{G, H\} = 0$ is a constant of motion.

3. Even more generally, for any function $G \in \mathcal{C}^\infty(U)$,

$$\frac{\mathrm{d}G(x(t))}{\mathrm{d}t} = \{G, H\}(x(t)).$$

Now, let us recall some properties of the time t flow of a differential equation which is Hamiltonian for (π, H), i.e. the map $\phi_t \colon x(0) \mapsto x(t)$, which is well-defined in a neighborhood of any $m \in \mathcal{U}$ for t small enough:

1. ϕ_t preserves π: $\pi(\phi_t(x)) = {}^t\nabla_x\phi_t(x) \cdot \pi(x) \cdot \nabla_x\phi_t(x)$, where $\nabla_x\phi_t(x)$ is the Jacobian of ϕ_t at x. It means that the flow of a Hamiltonian differential equation for (π, H) preserves the Poisson structure π.

2. The previous condition can also be stated as meaning that the pull-back map $f \mapsto \phi_t^* f$, i.e. the map assigning to a smooth function f the smooth function $f \circ \phi_t$, is a Lie algebra morphism, i.e.

$$\phi_t^*\{f, g\} = \{\phi_t^* f, \phi_t^* g\}$$

   for all functions f and g.

3. Item 1 above means in particular that the geometry of π is preserved. For instance if at the initial point $x(0)$, the matrix $\pi(x(0))$ has some given rank, it has this same rank at every point along the integral curve $x(t)$. Below, we will give a much stronger statement, using the notion of symplectic leaves.

Definition 2.1.3. A *symplectic singular foliation* on $\mathcal{U} \subset \mathbb{R}^n$ is a partition

$$\mathcal{U} = \bigcup_{c \in I} \mathcal{F}_c$$

by submanifolds, such that each $\mathcal{F}_c$ is equipped with a symplectic structure ω_c. The pair $(\mathcal{F}_c, \omega_c)$ is called a *symplectic leaf*.

Theorem 2.1.4 ([43, 65])**.** *Any Poisson structure on $\mathcal{U} \subset \mathbb{R}^n$ induces a natural foliation by symplectic leaves characterized by the following two properties:*

1. *two points belong to the same symplectic leaf if and only if they can be connected by a sequence of Hamiltonian trajectories, i.e. by integrating the equation* (2.5) *for some choice of Hamiltonian functions.*

2. *for every* $c \in I$*, the inclusion* $i \colon \mathcal{F}_c \hookrightarrow M$ *is a Poisson morphism.*

In addition, the tangent space of the symplectic leaf $\mathcal{F}_c$ *at a point* m *coincides with the image of the matrix* $\pi(m)$*.*

Remark 2.1.5. The last point of the previous statement means that the tangent space of a leaf at a point is given by all the possible Hamiltonian vector fields at this point. A leaf of a point is therefore locally generated by all integral curves of Hamiltonian differential equations.

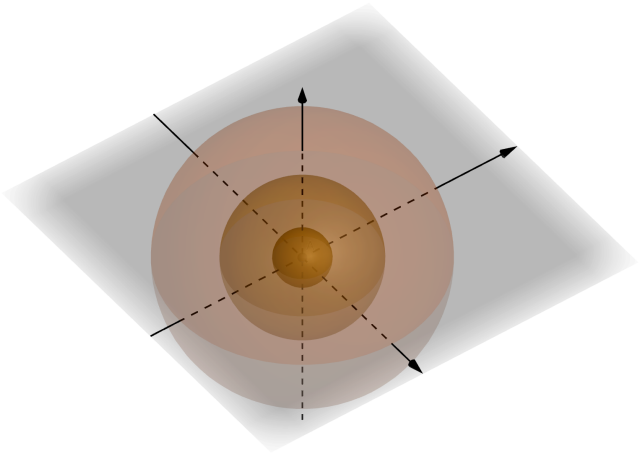


Figure 2.1: The symplectic foliation of $\mathbb{R}^3$ by concentric spheres and the origin associated to the canonical Poisson structure of $so(3)^*$

As observed in some of the following examples, the foliation is generically singular. Two neighbouring leaves do not necessarily have the same dimension and can differ from a topological point of view. Therefore, its study is an active field of research and motivates one of the long term applications of the numerical tools we present here.

The last reason explaining the importance of knowing that a differential equation is Hamiltonian for (π, H) is the following: by definition of a leaf, a solution $x(t)$ of a Hamiltonian differential equation for (π, H) can not "jump" from one symplectic leaf to another. We mean that if $x(0)$ belongs to a leaf $\mathcal{F}_c$, then the solution $x(t)$ belongs to the same leaf for every t.

Remark 2.1.6. This last "constraint" is maybe less studied for numerical methods than the previous ones, because when the Poisson structure is a symplectic one, it is not a constraint at all: the foliation contains only one leaf being the whole space. But for non-symplectic Poisson structures this is a very important feature to take into account.

In conclusion, for any Poisson structure π:

♢ for any first order autonomous differential equation which is Hamiltonian for (π, H), the Hamiltonian H is constant along any integral curve;

♡ each integral curve stays on the same symplectic leaf of the foliation defined by π;

♠ the flow of this differential equation preserves π, i.e. is a Poisson morphism;

♣ the converse is not necessarily true: preservation of π does not guarantee that the flow is Hamiltonian.

2.1.3 Examples of Hamiltonian equations – first candidates for integrators

The goal of what follows is to explain the logic behind the construction of numerical schemes that take into account the geometric features described above. We illustrate it on simple cases yet instructive examples.

Important examples of Poisson structures are the symplectic ones in their canonical form, e.g. where $\pi = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix}$. For those, a wide example of symplectic integrators are already available in the literature. One construction of such integrators uses the principle of symplectic Runge–Kutta schemes ([75]). For an integer s, said to be the *stage* of the method, it reads:

$$\begin{aligned} x_{n+1} &= x_n + \Delta t \sum_{i=1}^{s} b_i k_i \\ k_l &= \pi \cdot \nabla H(x_n + \Delta t \sum_{j=1}^{n} a_{lj} k_j) \quad \forall l \in [\![1, s]\!] \end{aligned} \tag{2.7}$$

where slopes k_i are implicitly defined and coefficients b_i and a_{ij} are chosen such that the discrete flow preserves π. We emphasize two features of this particular Poisson structure:

1. π is constant with respect to x,
2. any trajectory preserving it is necessary a time-dependent Hamiltonian one, at least locally, meaning that the map $\phi_{\Delta_t} \colon x_n \mapsto x_{n+1}$ is the flow of a non-autonomous (= time-dependent) Hamiltonian differential equation $\dot{y}(t) = \pi(y(t)) \cdot \nabla H_t(y(t))$.

For a Poisson structure π on a vector space given by a constant but degenerate skew-symmetric matrix, the same principle can be applied ([36]) and leads to a discrete flow that preserves the Poisson tensor, i.e. a Poisson integrator. However, even in that slight extension, it may lead to non-physical simulations, e.g. non-Hamiltonian Poisson integrators. A discrete trajectory does not necessarily stays on a symplectic leaf. Such a fact is due to existence of outer Poisson automorphisms, as illustrated in an example section 4.1.1. This remark motivates a theoretical and geometric approach to the question of Poisson integrators.

2.1.4 Hamiltonian Poisson integrators

Although the present work has many links with differential geometry, local coordinates are required for our construction of numerical integrators. That explains in most of the sections the use of open subsets of $\mathbb{R}^n$ rather than manifolds. The next definition follows this point of view.

Definition 2.1.7. We call *integrator* of order k for a differential equation

$$\dot{x}(t) = X(x(t))$$

a family of diffeomorphisms of the open subset[3] $\mathcal{U} \subset \mathbb{R}^n$

$$\phi_h \colon \mathcal{U} \longrightarrow \mathcal{U},$$

depending smoothly on a real parameter h such that the exact solution of the differential equation coincides with $\phi_h(x(0))$ up to order k in h, i.e. $\|\phi_h(x(0)) - x(h)\| = o\big(h^k\big)$. The *numerical scheme of timestep* Δt associated to an integrator consists in the recursive sequence

$$x_0 = x \text{ and } x_{n+1} = \phi_{\Delta t}(x_n).$$

Remark 2.1.8. Since a numerical scheme is defined by its iterations, the words *integrator*, *numerical method* and *numerical scheme* can be understood without ambiguity as synonyms all along this manuscript.

Consider now a differential equation as in (2.5) on $\mathcal{U} \subset \mathbb{R}^n$ which is Hamiltonian for a Poisson structure π and a Hamiltonian $H \in C^\infty(\mathcal{U})$.

Definition 2.1.9. An integrator of order k for the Hamiltonian differential equation (2.5)

$$\phi_h \colon \mathcal{U} \longrightarrow \mathcal{U},$$

is said to be a *Poisson integrator* if ϕ_h is a Poisson diffeomorphism of $(\mathcal{U}, \pi)$ for all h for which it is defined.

As explained in the Example 4.1.1, Poisson integrators can have a flow: the trajectories may jump from one symplectic leaf to another, and thus have non-physical behaviour. Hence, we formulate the following definition.

Definition 2.1.10. An integrator of order k for (2.5)

$$\phi_h \colon \mathcal{U} \longrightarrow \mathcal{U},$$

is said to be a *Hamiltonian Poisson integrator* of order $k \geqslant 1$ if there exists a time-dependent Hamiltonian function $(H_t)_t$, depending smoothly on t, that coincides with H up to order $k-1$, i.e. $H_t - H = o\big(t^{k-1}\big)$, and whose integral curve coincides with the curve $h \longrightarrow \phi_h(x)$ for all $x \in \mathcal{U}$ for which it is defined.

The following proposition claims that this second definition is strictly stronger.

Proposition 2.1.11. *A Hamiltonian Poisson integrator of order k is a Poisson integrator of order k.*

Proof. As long as it is well-defined, the flow of a time dependent Hamiltonian differential equation is a family of Poisson diffeomorphisms. Also, if H_t and H coincide up to order $k-1$, their Hamiltonian flows coincide then up to order k. □

Remark 2.1.12. As mentioned in the introduction, in general, we will not need in definition 2.1.10 to describe explicitly the family (H_t). All what matters at this point is that it exists.

[3]There is a subtle point here: we cannot assume ϕ_h to be a well-defined diffeomorphism from $\mathcal{U}$ to $\mathcal{U}$ for all h small enough, but we can assume that for all h small enough, there is an open subset $\mathcal{U}_h \subset \mathcal{U}$ on which ϕ_h is a diffeomorphism onto its image.

Backward analysis and modified Hamiltonian

Backward analysis is the theoretical explanation of the well-known good behaviour of symplectic integrators on long run simulations ([5]). For symplectic integrators, when one intends to approximate the trajectory of the Hamiltonian system coming from a Hamiltonian function H, each iteration in the discrete trajectory is the time h flow of a time-dependent Hamiltonian function $(H_t)_{t\in I}$. In good cases, there exists a Hamiltonian function $H(h)$ that does *not* depend on t whose time 1-flow coincides with the time h-flow of $(H_t)_{t\in I}$. Such a function $H(h)$ always exist at the formal level and is called *modified Hamiltonian.* Our definition of Hamiltonian Poisson integrator comes from this remark: indeed, a Hamiltonian Poisson integrator is a Poisson integrator admitting a modified Hamiltonian. We plan to keep on working on consequences of this property. A first attempt can be found later on with introduction of Magnus formula (2.5.2) that ensures the existence of a modified Hamiltonian, that is to say a formal Hamiltonian function defining the discrete trajectory of a Hamiltonian Poisson integrator.

To explain the notion of modified Hamiltonian, let us consider the general case of integrators, leaving Poisson structures aside at the moment. Let ϕ_h be an integrator of order k for a differential equation given by a vector field X as in definition 2.1.7. In general, the integrator ϕ_h will be the time h flow of a time dependent vector field $(X_t)_t$ (that coincides with X up to a given order). As proved in section IX.1 of [32], there exists a formal[4] vector field $X_h \in \mathfrak{X}(\mathcal{U})[[h]]$ that does not depend on the time t such that, formally[5]:

$$\phi_h = \Phi^1_{X_h}. \tag{2.8}$$

In words, the time 1-flow of the formal vector field X_h is ϕ_h. We are looking for an equivalent of this formal vector field X_h in the context of Hamiltonian Poisson integrators.

Definition 2.1.13 (Modified Hamiltonian of a Hamiltonian Poisson integrator)**.** Let $(H_t)_t$ be the time-dependent Hamiltonian function of a given Hamiltonian Poisson integrator ϕ_h. We call modified Hamiltonian a formal series $H_h \in \mathcal{C}^\infty(\mathcal{U})[[h]]$ such that ϕ_h coincides, formally in h, with the time 1-flow of H_h.

Equivalently, this definition means that the time 1-flow of

$$X_h = \pi \cdot \nabla H_h. \tag{2.9}$$

coincides with the Hamiltonian Poisson integrator ϕ_h formally in h.

Remark 2.1.14.

1. As stated in [32], symplectic integrators always admit a modified Hamiltonian. However, it is not true anymore for a generic Poisson structure: an integrator preserving it may not admit such a backward analysis. Related issues are illustrated example 4.1.1 and lead us to the notion of Hamilton Poisson integrator.

2. The modified Hamiltonian is not unique: adding a Casimir function to H_h does not change equation (2.9).

[4] We mean by that a formal series in h with coefficients in $X(\mathcal{U})$.

[5] The flow $\Phi^1_{X_h}$ of X_h at time 1 is defined as $\Phi^1_{X_h} = \exp X_h = \sum_{k\in\mathbb{N}} \frac{h^k}{k!}(X_h)^k$, where X_h is seen as an endomorphism of $\mathcal{C}^\infty(\mathcal{U})[[h]]$. By definition, equation (2.8) can then be rephrased as: for any $f \in \mathcal{C}^\infty(\mathcal{U})$, $f(\phi_h) = \exp X_h(f)$ in $\mathcal{C}^\infty(\mathcal{U})[[h]]$.

As we will see in Section 2.5.2, and as will be detailed in Section 3.1, there is a way to compute a modified Hamiltonian function provided that the time-dependent Hamiltonian functions (H_t) are given: *A modified Hamiltonian of a given Hamiltonian Poisson integrator is obtained by applying Magnus formula to the time dependent Hamiltonian function $(H_t)_t$ that defines the Poisson integrator.*

2.2 Bi-realisations for Poisson manifolds

Having set the preliminaries and the framework in the previous sections, we are now ready to address the core of the thesis: construct Hamiltonian Poisson integrators for a wide class of Poisson structures and any Hamiltonian differential equation on them. One of the important "tools" for the procedure is the notion of local symplectic groupoid associated to a Poisson structure that arose in [16]. See [18] for a modern introduction to the matter. Notice that we will mostly not need the whole groupoid structure but a neighborhood of the identity of the latter, which can be considered to be closer from the version of [37]. Several authors [26], [23] (to cite a few) have already used symplectic groupoids[6] to construct some numerical integrators: the relation is explained in [13].

Symplectic groupoids of Poisson manifolds are not easy to construct as an object, even while our method does not use all the structure of the Lie groupoid (product, inverse) but only the source and target. All we need is what we call a *bi-realisation*, so we will not have to define the notion of symplectic groupoid in full generality. We will explain below the need of this new terminology.

In the first subsections of what follows, we explain under which circumstances this bi-realisation, whose existence is guaranteed by theoretical arguments, is explicitly constructable. Then, we detail how to construct a decent Poisson integrator for the differential equation (2.5) at order 1 and of time-step h. For this we just use the subset $\{(x, h\nabla H(x)), x \in \mathcal{U}\}$ or geometrically: the graph of $h\mathrm{d}H$ in T^*M. It is moreover possible to get a better Poisson integrator at an arbitrary order by replacing $h\nabla H$ by a polynomial in h, of the form $h\nabla H + \frac{h^2}{2}\nabla S_2 + \dots$, whose terms are computed by an easy recursion, solving Hamilton-Jacobi equation at the desired order. Details are developed at the beginning of section 2.4 and in section 2.5.1 where the Farmer theorem is explained. The modified Hamiltonian is also computed by a recursion through Magnus formula.

Existence of such bi-realisation is guaranteed by theorems, see [13] for details. Since it matters in what follows, we will systematically make remarks on what is computable and with what precision.

2.2.1 Bi-realisations I: definition and existence

The reader used to Poisson geometry may ask why we introduce below the concept of a bi-realisation, since she or he will probably understand immediately that those are in fact the local model of a symplectic groupoid. We insist in thinking that introducing the notion is conceptually clearer and makes our theory easier to understand for a public that has never heard about Lie groupoid. We start with an even more basic definition:

Definition 2.2.1. A *bi-surjection* is the following data:

[6] A Lie groupoid over a manifold, roughly speaking, is an analog of a Lie group, where to each element one associate two mappings to this base manifold: source α and target β. Then two elements are composable when the source of one matches the target of the other, and for those the standard group axioms are satisfied. The symplectic form is compatible with this composition. See for instance [65].

1. an open subset $\mathcal{U} \subset \mathbb{R}^n$ – the *phase space*,

2. an open subset $\mathcal{W} \subset \mathcal{U} \times \mathbb{R}^n$ containing $\mathcal{U} \times \{0\}$,

3. two surjective submersions, called *source* and *target*, $\alpha, \beta \colon \mathcal{W} \to \mathcal{U}$ such that for all $x \in \mathcal{U}$

$$\alpha(x, 0) = \beta(x, 0) = x.$$

We denote a bi-surjection by $(\mathcal{W}, \alpha, \beta)$.

Bi-surjections allow to associate a diffeomorphism of $\mathcal{U}$ out of any *bi-section*, i.e. any submanifold L of dimension n in $\mathcal{W}$ to which the restrictions of the source α and the target β are diffeomorphisms onto $\mathcal{U}$. A bi-section L of a bi-surjection $(\mathcal{W}, \alpha, \beta)$ induces a diffeomorphism $\varphi_L \colon \mathcal{U} \longrightarrow \mathcal{U}$ defined as $\varphi_L = \beta \circ (\alpha_{|_L})^{-1}$ as on figure 2.2.

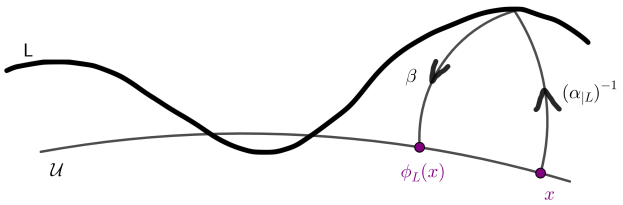


Figure 2.2: The diffeomorphism φ_L induced by a bi-section L of $\mathcal{W}$

The crucial remark is that, if L and $(\mathcal{W}, \alpha, \beta)$ are explicitly known, then the computation φ_L only requires to invert a diffeomorphism. This operation, in general, can be done numerically with required precision and with reasonable cost, so that the diffeomorphism φ_L can be easily computed. The discretisations that we are going to construct are families $(\varphi_{L_h})_h$ of diffeomorphisms, depending on a "small" real parameter h, associated to a family L_h of bi-sections such that $L_0 = \mathcal{U} \times \{0\}$, so that $\varphi_{L_0} = \mathrm{Id}_{\mathcal{U}}$ is the identity map.

Assume that $\mathcal{W} \subset \mathbb{R}^n \times \mathbb{R}^n$ comes equipped with a symplectic structure:

$$\omega := \sum_{i=1}^{n} dp_i \wedge dx_i \tag{2.10}$$

with $x_1, \ldots, x_n, p_1, \ldots, p_n$ being the natural variables on $\mathcal{U} \times \mathbb{R}^n$, labeled in that order. The corresponding Poisson structure satisfies:

$$\{x_i, x_j\}_\omega = \{p_i, p_j\}_\omega = 0 \text{ and } \{x_i, p_j\}_\omega = \mathbb{1}_{i=j}.$$

We can now state the main definition:

Definition 2.2.2 (Bi-realisation)**.** Let π be a Poisson structure on an open subset $\mathcal{U} \subset \mathbb{R}^n$. A bi-realisation of $(\mathcal{U}, \pi)$ is a bi-surjection $(\mathcal{W}, \alpha, \beta)$, with source α and target β satisfying the following:

1. α is a Poisson map,

2. β is an anti-Poisson map,

3. the fibers of α and β are symplectically orthogonal to each other.

In all three items above, $\mathcal{W}$ comes equipped with the Poisson bracket $\{\cdot,\cdot\}_\omega$ associated to the symplectic structure (2.10).

This definition can be compared with definition 3.3.3 in a more geometric context.

Remark 2.2.3. Conditions 1 – 3 in Definition 2.2.2 mean that for all functions $F, G \in C^\infty(\mathcal{U})$:

$$\alpha^*\{F,G\}_\pi = \{\alpha^*F, \alpha^*G\}_\omega, \quad \beta^*\{F,G\}_\pi = -\{\beta^*F, \beta^*G\}_\omega,$$

$$\{\alpha^*F, \beta^*G\}_\omega = 0.$$

Remark 2.2.4.

1. Closely related concepts are found in the literature, for instance the one of connected strict dual pairs ([16]). However, for our purpose, it matters that the symplectic form on the open subset $\mathcal{W}$ is the canonical one.

2. Last cited reference explains how to recover the groupoid multiplication out of source and target of a symplectic groupoid, see prop 1.2 of chapter 3. As a consequence, even if we do not use multiplication and inverse here, we can recover them from the data of a bi-realisation of a Poisson structure.

We will quote the following three results, for completeness and future references.

Lemma 2.2.5. *For every $F \in C^\infty(\mathcal{U})$:*

$$\{(x_1,\dots,x_n,\partial_{x_1}F,\dots,\partial_{x_n}F), (x_1,\dots,x_n) \in \mathcal{U}\}$$

is a Lagrangian submanifold of $\mathcal{U}\times\mathbb{R}^n$ equipped with the canonical symplectic structure ω.

Proposition 2.2.6. *Let $(\mathcal{W},\alpha,\beta)$ be a bi-realisation for a Poisson structure π on $\mathcal{U}$. For any bi-section $L\subset\mathcal{W}$ which is Lagrangian with respect to ω, the induced diffeomorphism $\varphi_L\colon\mathcal{U}\longrightarrow\mathcal{U}$ is a Poisson diffeomorphism. Moreover, for Lagrangian bi-sections contained in some neighborhood of $\mathcal{U}\times\{0\}$, this Poisson diffeomorphism is the value at time 1 of the flow of a time-dependent Hamiltonian vector field.*

As a consequence, for every $F \in C^\infty(\mathcal{U})$ a small enough function[7] the Lagrangian submanifold

$$\{(x_1,\dots,x_n,\partial_{x_1}F,\dots,\partial_{x_n}F), (x_1,\dots,x_n) \in \mathcal{U}\} \subset \mathcal{W}$$

is a Lagrangian bi-section of $(\mathcal{W},\alpha,\beta)$. The following result is now classical in the theory of symplectic Lie groupoid:

Theorem 2.2.7 (Existence and uniqueness)**.** *[37, 16] Any Poisson structure on an open subset $\mathcal{U}\subset\mathbb{R}^n$ admits a bi-realisation. Furthermore, it is canonical in the following sense: two different bi-realisations of a Poisson structure are symplectomorphic through some symplectomorphism fixing $\mathcal{U}\times\{0\}$, at least in a neighborhood of the latter.*

[7] More precisely, the ∞-norm of the derivative at a point must be smaller than some local bound.

2.2.2 Bi-realisations II: Explicit constructions

Theorem 2.2.7 states that bi-realisations do exist and are unique. Below we explain two tools to construct such: Poisson spray for a generic Poisson structure and cotangent lift for the Poisson structure of the dual of a Lie algebra. They are respectively illustrated in the present manuscript on the Poisson bracket $\{x_i, x_j\} = a_{ij}x_ix_j$ (see equation (2.13)) related to Lotka-Volterra systems coming from population dynamics and the Poisson bracket on $so^*(n)$ (see equation (2.15)) related for $n = 3$ to rigid body dynamics. A third construction of bi-realisation is due to Karasev and is described in theorem 2.2.17.

Poisson Spray and Moser's trick

We give here a conceptual approach to the construction of bi-realisation using the notion of Poisson spray.

Definition 2.2.8 ([19])**.** Let (M, π) be a Poisson manifold, $\tau\colon T^*M \to M$ the cotangent projection and for λ a non-zero real number, $m_\lambda\colon \xi \in T^*M \mapsto \lambda\xi \in T^*M$ the fiberwise multiplication by λ. A vector field $X \in \mathfrak{X}(T^*M)$ is said to be a Poisson spray if it verifies the following two conditions:

1. $\forall \xi \in T^*M$, $\mathrm{d}_\xi\tau.X(\xi) = \pi^\#(\xi)$,
2. X is homogeneous of degree 1: $\forall \lambda \in \mathbb{R}^*$, $\mathrm{m}_\lambda^* X = \lambda X$.
   i.e. $\mathrm{d}_{\lambda\xi} m_{\lambda^{-1}}.X(\lambda\xi) = \lambda X(\xi)$.

Example 2.2.9. For some choice of coordinates x_i, the Poisson tensor has the form

$$\pi(x) = \sum_{1\leqslant i<j\leqslant n} \pi_{ij}(x)\partial_{x_i} \wedge \partial_{x_j}.$$

Denoting (x, ξ) the induced cotangent coordinates,

$$X(x,\xi) = \sum_{1\leqslant i<j\leqslant n} \pi_{ij}(x)\xi_j\partial_{x_i}$$

is a Poisson spray. The homogeneity is easily seen by looking at the linearity in ξ.

The second point of its definition implies that X vanishes on the zero section 0_{T^*M}. Consequently, there exists a neighborhood $\mathcal{W}$ of 0_{T^*M} such that the time 1 flow of X $\Phi_X^1\colon \mathcal{W} \to \Phi_X^1(\mathcal{W})$ is a well-defined global diffeomorphism onto its image.

Remark 2.2.10. For a given Poisson structure, Poisson sprays always exist (see [19]). However, Poisson sprays are far from being unique. For instance, one can add a term of the form "$f(x)\xi_i\xi_j\partial_{\xi_j}$" to it – this is an important freedom that allows to construct explicit integration of the flow above in a lot of important cases.

Theorem 2.2.11 ([19])**.** *Any Poisson spray induces target, source and multiplicative form of the local symplectic groupoid near 0_{T^*M} in the following way :*

1. $\bar{\alpha} = \tau\colon T^*M \to M$,
2. $\bar{\beta} = \tau \circ \Phi_X^1$,

3. $\Omega = \int_0^1 {\Phi_X^s}^* \omega \, ds$*, where* ω *is the canonical symplectic form.*

Note that Ω is symplectic up to shrinking of $\mathcal{W}$. Also, it is *not* necessarily the canonical symplectic form ω used in the definition of bi-realisation. However, by the so-called Moser's trick, a Poisson spray can be "rectified" to yield a bi-realisation. So in short the following result is often instrumental for the final construction:

Theorem 2.2.12. *Any Poisson spray gives a symplectic open subset which is symplectomorphic to a bi-realisation.*

Proof. As mentioned, by Moser's trick [73], the canonical symplectic form ω and the 2-form Ω of the Poisson spray are symplectomorphic in a neighborhood of the zero section in T^*M: $\omega = \psi^*\Omega$. Moreover, ψ is the identity map on $M \subset T^*M$, and so is its differential at any point of M. Then, a bi-realisation on this neighborhood is given by:

$$\alpha = \psi^* \bar{\alpha}, \quad \beta = \psi^* \bar{\beta}.$$

□

For a generic Poisson structure, the flow Φ_X of a Poisson spray may not be explicitly computable. However:

Corollary 2.2.13. *If both the Poisson spray and the Moser symplectomorphism are explicitly computable, then theorem 2.2.12 gives an explicit bi-realisation.*

Dual of a Lie algebra: cotangent lifts

In the case of the linear Poisson structure on the dual of a Lie algebra, there is a direct way of constructing bi-realisations.

Proposition 2.2.14. *Let* $\mathfrak{g}$ *be a Lie algebra of a Lie group* G*, and* $\varphi \colon G \to \mathfrak{g}$ *a local diffeomorphism in* 1_G*, bijective on an open subset* $\mathcal{V}$ *containing the unit* 1_G*, such that :*

1. $\varphi(1_G) = 0$
2. $T_{1_G}\varphi = Id.$

Let us denote by ψ *the inverse of* φ *and* $\bar{\mathcal{V}} = \varphi(\mathcal{V})$.
Then a bi-realisation of the Lie-Poisson structure on $\mathfrak{g}^*$ *is given by:*

$$\begin{cases} \alpha \colon \bar{\mathcal{V}} \times \mathfrak{g}^* \to \mathfrak{g}^* : (\eta, \xi) \mapsto R^*_{\psi(\eta)} \left(T^*_{\psi(\eta)} \varphi \right) .\xi \\ \beta \colon \bar{\mathcal{V}} \times \mathfrak{g}^* \to \mathfrak{g}^* : (\eta, \xi) \mapsto L^*_{\psi(\eta)} \left(T^*_{\psi(\eta)} \varphi \right) .\xi = Ad^*_{\psi(\eta)} . \alpha(\eta, \xi) \end{cases} .$$

Let us describe more precisely these source and target maps. Since φ maps $\mathcal{V} \subset G$ to $\bar{\mathcal{V}} \subset \mathfrak{g}$, its differential $T\varphi$ maps $T\mathcal{V}$ to $T\bar{\mathcal{V}} \simeq \bar{\mathcal{V}} \times \mathfrak{g}$. Composing this map with the right and left identifications of $T\mathcal{V}$ with $\mathcal{V} \times \mathfrak{g}$ and using the diffeomorphism ψ, one gets two families indexed by $\eta \in \bar{\mathcal{V}}$ of linear invertible endomorphisms of $\mathfrak{g}$. The source and targets above are the dual of these maps[8]. The example of $so(n)^*$ is detailed in section 2.2.3 while mathematical precisions can be found in the example 3.3.7.

[8]The reader familiar with the notion of *logarithmic derivative* will notice that those maps are the inverse of the dual of the logarithmic derivative of ψ after right and left trivialisations of TG.

Remark 2.2.15. Notice that we do not assume φ to be the logarithm, i.e. the inverse of the exponential map. It may be any local diffeomorphism. In fact, the logarithm map may not be a good choice since its differential may be too complicated to compute at each iteration of our future numerical method.

Corollary 2.2.16. *If φ, its inverse and its differential are explicitly computable, then proposition 2.2.14 gives an explicit bi-realisation.*

A remark on Karasev construction

Several methods to construct explicit bi-realization of a Poisson structure will be given in Section 2.2.3, in particular for constant, linear, and some quadratic Poisson structures. We indicate here a general method that may also be applied, that predates in construction of the symplectic groupoid and is due to Karasev [37].

Let $(\mathcal{U}, \pi)$ be a Poisson manifold, with $\mathcal{U}$ a subset of $\mathbb{R}^n$, so that $T^*\mathcal{U}$ can be identified with pairs $m \in \mathcal{U}$ and $\xi \in \mathbb{R}^n$. Let ∇ be the canonical affine connection. For every $\xi \in \mathbb{R}^n$, consider the integral curve $m(t)$ of the differential equation:

$$\dot{m}(t) = \pi^{\#}_{m(t)}\xi \text{ and } m(0) = m.$$

We denote the corresponding flow by $(m, \xi, s) \longrightarrow \Xi(m, \xi)^{(s)}$ for every $m \in \mathcal{U}, \xi \in \mathbb{R}^n, s \in \mathbb{R}$ for wih the solution is well-defined and call it the *Poisson geodesic flow*.

The idea of Karasev consists in looking at the following two equations whose unknowns α, β are in M, for a given $(m, \xi) \in T^*M$:

$$\int_0^1 \Xi(\alpha, \xi)(t)dt = m \text{ and } \int_{-1}^0 \Xi(\beta, \xi)(t)dt = m.$$

Since, for $\xi = 0$, the unique solutions are $\alpha = \beta = m$, there exists a neighborhood $\mathcal{W}$ of M in T^*M on which the two previous equation have a unique solution, defining therefore two maps $\mathcal{W} \to M$ that we denote α and β. Moreover, he proves the following theorem:

Proposition 2.2.17 ([37])**.** *The triple $(\mathcal{W}, \alpha, \beta)$ is a bi-realisation for a Poisson structure (M, π).*

Remark 2.2.18. This bi-realisation is explicit provided that the Poisson geodesic flow Ξ and its integral can be computed. It is computable by quadratures if so is the geodesic flow, which is the case for a large class of Poisson structures. However, we have not been able to find an example where Karasev construction leads to explicit bi-realizations that we are not able to construct by simpler means.

2.2.3 Examples of explicit bi-realisations

In what follows we construct a symplectic bi-realisation for several classes of Poisson structures, using various techniques, including Poisson sprays. We start with the simplest Poisson structure given by a symplectic form written in canonical (Darboux) coordinates, to recover some symplectic integrators. Then we continue with a couple of constructions that will later be used in the numerical tests.

Symplectic case.

Let $M = \mathbb{R}^2 = \{(q,p)\}$, then $\pi = \partial_p \wedge \partial_q$. Let (q,p,ξ_q,ξ_p) be cotangent coordinates on $\mathbb{R}^4$. Consider a Poisson spray $X(q,p,\xi_q,\xi_p) = \xi_p\partial_q - \xi_q\partial_p$.
The objects of theorem 2.2.11 are:

1. $\bar{\alpha}\colon T^*M \to M\colon q,p,\xi_q,\xi_p \mapsto (q,p)$,
2. $\bar{\beta}\colon T^*M \to M\colon q,p,\xi_q,\xi_p \mapsto (q+\xi_p, p-\xi_q)$,
3. $\Omega = \omega + \frac{1}{2}\mathrm{d}p \wedge \mathrm{d}\xi_p - \frac{1}{2}\mathrm{d}\xi_q \wedge \mathrm{d}q - \frac{1}{3}\mathrm{d}\xi_q \wedge \mathrm{d}\xi_p$.

The symplectomorphism announced by theorem 2.2.12 between Ω and the canonical symplectic structure ω is given by

$$\Psi\colon \begin{pmatrix} q \\ p \\ \xi_q \\ \xi_p \end{pmatrix} \mapsto \begin{pmatrix} q - \frac{\xi_p}{2} \\ p + \frac{\xi_q}{2} \\ \xi_q \\ \xi_p \end{pmatrix},$$

and the resulting bi-realisation is $\mathcal{W} = \mathbb{R}^2 \times \mathbb{R}^2$ with structural maps

$$\begin{cases} \alpha\colon (q,p,\xi_q,\xi_p) \mapsto (q - \frac{1}{2}\xi_p, p + \frac{1}{2}\xi_q) \\ \beta\colon (q,p,\xi_q,\xi_p) \mapsto (q + \frac{1}{2}\xi_p, p - \frac{1}{2}\xi_q) \end{cases}. \tag{2.11}$$

Remark 2.2.19. Since bi-realisations will be used to construct numerical schemes preserving the Poisson structure, the bi-realisation (2.11) will provide symplectic integrators. In general, they will be different from the existing ones.

Quadratic Poisson structures

The following example will be important for Lotka-Volterra systems. Consider $M = \mathbb{R}^n$ and a quadratic Poisson structure:

$$\pi = \sum_{1 \leqslant i,j \leqslant n} a_{ij} x_i x_j \partial_{x_i} \wedge \partial_{x_j} \tag{2.12}$$

Using the (natural) Poisson spray of [46]:

$$X = \sum_{1 \leqslant i,j \leqslant n} a_{ij} x_i x_j \xi_i \partial_{x_j} - \sum_{1 \leqslant i,j \leqslant n} a_{ij} x_i \xi_i \xi_j \partial_{\xi_j},$$

and the Moser symplectomorphism:

$$\Psi\colon \begin{pmatrix} x_j \\ p_j \end{pmatrix} \mapsto \begin{pmatrix} e^{-\frac{1}{2}\sum_i a_{ij} x_i p_i} x_j \\ e^{\frac{1}{2}\sum_i a_{ij} x_i p_i} p_j \end{pmatrix},$$

one constructs the following bi-realisation: $W = \mathbb{R}^n \times \mathbb{R}^n$ and

$$\begin{cases} \alpha\colon (x,p) \mapsto \left(e^{-\frac{1}{2}\sum_i a_{ij} x_i p_i} . x_j \right)_{j=1,\ldots,n} \\ \beta\colon (x,p) \mapsto \left(e^{\frac{1}{2}\sum_i a_{ij} x_i p_i} . x_j \right)_{j=1,\ldots,n} \end{cases}. \tag{2.13}$$

Canonical Poisson structure on $so^*(n)$

Let us spell-out the cotangent lift construction in the case of the algebra $so(n)$ of anti-symmetric matrices. The scalar product $< .,. >: (X,Y) \in so(n) \mapsto \mathrm{Tr}(X^T.Y) \in \mathbb{R}$ induces an isomorphism between $so(n)$ and its dual. The local diffeomorphism we use is the Cayley transform, from the connected component of Id in $SO(n)$ to $so(n)$:

$$\varphi\colon SO(n)_+ \to so(n)\colon Q \mapsto 2\frac{Q-I}{Q+I} \tag{2.14}$$

with inverse

$$\psi\colon so(n) \to SO(n)_+\colon A \mapsto \frac{2+A}{2-A}.$$

Its derivative at $Q \in SO(n)_+$ is

$$T_Q\varphi\colon so(n) \to so(n)\colon H \mapsto 2(I+Q^{-1})^{-1}.H.(I+Q)^{-1}$$

and the transpose of it by $< .,. >$ is its cotangent lift $T^*\varphi$. Using that for all $(B,H) \in so(n)^2$, $< B, T_Q\varphi.H >=< 4(I+Q)^{-1}B(I+Q^{-1})^{-1}, H >$ and setting $Q=\psi(A)$, $A \in so(n)$, one gets

$$\begin{array}{rccc} T^*\varphi\colon & so(n)\times so(n)^* & \to & SO(n)\times so(n) \\ & (A,x) & \mapsto & (\psi(A), (I+\frac{A}{2}).x.(I-\frac{A}{2}). \end{array}$$

Since the metric is Ad-invariant, $\mathrm{Ad}^*_Q x = Q.x.Q^{-1}$. We can choose $\mathcal{W} = so(n)\times so(n)$ and the source and target:

$$\left\{ \begin{array}{l} \alpha\colon so(n)\times so(n) \to so(n)\colon (A,x) \mapsto (I+\frac{A}{2}).x.(I-\frac{A}{2}) \\ \beta\colon so(n)\times so(n) \to so(n)\colon (A,x) \mapsto (I-\frac{A}{2}).x.(I+\frac{A}{2}) \end{array} \right. . \tag{2.15}$$

In conclusion, the construction of numerical schemes requires explicit objects, so that computations can be made. The notion of bi-realisation of section 2.2.2 provides such a framework. The next section explains how we use those bi-realisation to construct Hamiltonian Poisson integrators.

2.3 Geometry of Lagrangian bi-sections

We explain here the differential geometry that leads to Hamilton-Jacobi equation. Those geometric tools rely on some calculus on Lagrangian bi-sections of a bi-realisation. A differential geometry vocabulary and the proofs will be either explained all along or detailed in chapter 3, see also [13].

2.3.1 A canonical correspondence

The main result is a canonical correspondence between smooth families of Lagrangian bi-sections of $\mathcal{W}$ and smooth families of closed 1-forms on $\mathcal{U}$.

Let I be a real open interval containing 0 and $\xi \in \mathcal{C}^\infty(I, \Omega^1_0(\mathcal{U}))$ a smooth family of closed 1-forms on $\mathcal{U}$. Let L_0 be a Lagrangian bi-section of $\mathcal{W}$. There exists an unique vector field $\overrightarrow{\xi}$ on $\mathcal{W}$ such that

$$\omega(\overrightarrow{\xi}, \cdot) = \alpha^*\xi.$$

One side of the previously cited correspondence is the following observation:

Proposition 2.3.1. *Let $\xi \in \mathcal{C}^\infty(I, \Omega^1_0(\mathcal{U}))$ be a smooth family of closed 1-forms on $\mathcal{U}$ and assume that for all $t \in I$, the flow of $\Phi^t_{\overrightarrow{\xi}}$ is well-defined on L_0. Consider the following family of submanifolds of $\mathcal{W}$:*

$$L_t = \Phi^t_{\overrightarrow{\xi}}(L_0) \tag{2.16}$$

Then $\mathscr{L} = (L_t)_{t\in I}$ is a smooth family of Lagrangian bi-sections.

Remark 2.3.2. Upon identifying $\mathcal{W}$ with the local symplectic groupoid integrating π, the vector field $\overrightarrow{\xi}$ corresponds to the left action of the Lie algebroid $T^*\mathcal{U}$ on it.

For a smooth family of Lagrangian bi-sections $\mathscr{L} = (L_t)_t$, there exists a unique[9] smooth family of closed 1-forms $\xi_{\mathscr{L}}$ on $\mathcal{U}$ such that (2.16) holds. $\xi_{\mathscr{L}}$ is called the *variation form* of $\mathscr{L}$. We give a brief construction here.

Let $x \in L_0$ and $\gamma\colon I \to \mathcal{W}$ be a path such that $\gamma(t) \in L_t$ for all t. Then, since L_0 is Lagrangian :

$$\begin{aligned} \dot\gamma(0) &\in T_{|L_0}\mathcal{W} \\ [\dot\gamma(0)] &\in N_{|L_0}L_0 = {}^{T_{|L_0}\mathcal{W}}\!/_{TL_0} \simeq T^*L_0 \end{aligned}$$

so that we get a covector on L_0 at x. This covector actually only depends on the family $\mathscr{L}$: any other $\tilde\gamma$ such that $\tilde\gamma(t) \in L_t$ for all t has the same normal projection. Moreover, the same reasoning can be done replacing L_0 by L_t for any $t \in I$ and those covectors glue along while the starting point $\gamma(0)$ varies. At this stage, we obtained a family $(\hat\xi_t)_t$ of 1-forms such that for each $t \in I$:

$$\hat\xi_t \in \Omega^1(L_t).$$

Two remarks conclude the construction :

1. since L_t is Lagrangian, $\mathrm{d}\hat\xi_t = 0$,
2. since L_t is a bi-section, the source induces by push-forward a diffeomorphism from $\Omega^1(L_t)$ to $\Omega^1(\mathcal{U})$.

The resulting smooth family of closed 1-forms ξ is the desired variation form of $\mathscr{L}$. The previous reasoning can be done in a general local symplectic groupoid of a Poisson manifold (M, π), hence the:

Theorem 2.3.3. *Let I be an interval containing 0. In a symplectic groupoid $\mathcal{G} \rightrightarrows M$ endowed with its symplectic form Ω, there is a canonical one-to-one correspondence between:*

(i) smooth families of Lagrangian bi-sections $(L_t)_{t\in I}$ of $(\mathcal{G}, \Omega)$,

(ii) pairs made of a Lagrangian bi-section L_0 and a smooth family of closed one-forms on the base $(\xi_t)_{t\in I}$ such that the vector field $\pi^\#(\xi_t)$ is a complete vector field on M.

2.3.2 The Hamilton-Jacobi equation

Two examples of smooth families of Lagrangian bi-sections in a bi-realisation $\mathcal{W}$ matter in view of applying theorem (2.3.3).

[9] up to a well-known cornelian dilemma between right and left

Example 2.3.4.

- Let $H \in \mathcal{C}^\infty(\mathcal{U})$ be a Hamiltonian. It is classical (see also appendix .1) that $\mathscr{L}_H = (\Phi^t_{\alpha^* H})_{t\in I}$ induces the flow of H on $\mathcal{U}$:

$$\text{if } L_t = \Phi^t_{\alpha^* H}(\mathcal{U}),\ \varphi_{L_t} = \Phi^t_H.$$

- Explicit families of Lagrangian bi-sections are obtained by graphs of smooth families of closed forms on $\mathcal{U}$ $(\zeta_t)_t \in \Omega^1_0(\mathcal{U})$: $\mathscr{L}^\zeta = (\{\zeta_t(x),\ x \in \mathcal{U}\})_t$. This is the geometric (closed forms replace gradients) and dynamical (there is a time parameter t) reformulation of lemma 2.2.5.

Apart from Hamiltonian Poisson integrators we aim at constituting, the context yields a natural question: how to interpolate the Hamiltonian flow with a time-dependent family of closed 1-forms, i.e. how to choose ζ_t such that

$$\mathscr{L}^\zeta = \mathscr{L}_H\ ? \tag{2.17}$$

(2.17) implies the exactness of $\zeta_t : \zeta_t = \mathrm{d}S_t$ and the answer is given by their equality of variation form. Since it is an equality of exact 1-forms :

$$\mathrm{d}\frac{\mathrm{d}S_t}{\mathrm{d}t}(x) = \mathrm{d}\alpha^* H\left(\Phi^t_{\alpha^* H}(x)\right) \tag{2.18}$$

$$\frac{\mathrm{d}S_t}{\mathrm{d}t}(x) = \alpha^* H\left(\mathrm{d}_x S_t\right) + c(t) \tag{2.19}$$

where $c(t)$ is a time-dependent constant resulting from integration. We set $c(t) = 0$ and obtain the Hamilton-Jacobi equation

$$\begin{cases} \frac{\mathrm{d}S_t}{\mathrm{d}t}(x) & = \alpha^* H\left(\mathrm{d}_x S_t\right) \\ S_0 & = 0 \end{cases} \tag{2.20}$$

We can now state one of our main result:

Theorem 2.3.5. *Assume we are given $(\mathcal{W}, \alpha, \beta)$ a bi-realisation of a Poisson structure $(\mathcal{U}, \pi)$ and H a Hamiltonian function.*

1. *The Hamilton-Jacobi equation* (2.20) *admits a solution $(S_t)_t$ in a neighborhood of $M \times \{0\} \subset \mathcal{U} \times \mathbb{R}$.*
2. *The family of Poisson automorphisms induced by the Lagrangian bi-sections given by the graphs of the $(dS_t)_t$ is the flow of H.*

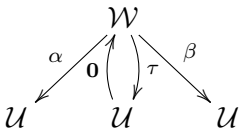
Remark 2.3.6. Since bi-realisations are symplectomorphic to neigborhoods of the identity in a symplectic groupoid, the previous construction justifies the following motto :
The local groupoid of a Poisson structure is the space in which Lagrangian perturbations of the identity section recover the foliation on the base.
Given a bi-realisation, Hamilton-Jacobi equation tells exactly in which manner.

2.4 Explicit construction of Hamiltonian Poisson integrators

We are now ready to put together all what has been discussed in the context of Poisson geometry in the previous sections, and make the final step to construction of the appropriate structure preserving

integrators. To sum it up, we start with a Poisson structure π defined on an open subset $\mathcal{U} \subset \mathbb{R}^n$. The only assumption that we need is that it admits an *explicit* bi-realisation $(\mathcal{W}, \alpha, \beta)$.

We recall that $\mathcal{W}$ is an open subset of $\mathcal{U} \times \mathbb{R}^n$ containing $\mathcal{U} \times \{0\}$ equipped with its canonical symplectic structure. We denote its source by α, its target by β, and its base map by τ. It is consequently equipped with its canonical symplectic structure. We denote by $\mathbf{0} : \mathcal{U} \to \mathcal{W}$ the map $\mathbf{0}(x) = (x, 0)$.



Remark 2.4.1. We recall that for any $(x, p) \in \mathcal{W}$, $\alpha(x, p)$ and $\beta(x, p)$ are in the same symplectic leaf of π. This leaf is not necessarily the same symplectic leaf at the one containing $\tau(x, p) = x$.

Consider again the Hamiltonian differential equation

$$\dot{x}(t) = \pi(x(t)) \cdot \nabla H(x(t)) \tag{2.21}$$

for some Hamiltonian $H \in C^\infty(\mathcal{U})$.

We claim that we can construct an explicit Hamiltonian Poisson integrator of order k for (2.21). There are several steps that we now present.

Step 1. To start with, one needs to compute the first k terms of the *Hamilton-Jacobi transform* of H. The latter is a formal series with coefficients being smooth functions on $\mathcal{U}$ of the form

$$\mathcal{S}_t(H)(x) = tS_1(x) + \frac{t^2}{2}S_2(x) + \frac{t^3}{6}S_3(x) + \dots,$$

and the coefficients are computed by recursion as follows:

(a) Set $S_1(x) = H(x)$.

(In particular, for $k = 1$, the truncation of the generating transform of $H(x)$ is simply $tH(x)$.)

(b) The smooth function $S_{i+1}(x)$ is then given by the recursive formula:

$$S_{i+1}(m) = \left.\frac{d^i}{dt^i}\right|_{t=0} H\left(\alpha\left(d_m S_t^{(i)}\right)\right) \tag{2.22}$$

where we write $S_t^{(i)} = \sum_{j=1}^{i} \frac{t^j}{j!} S_j$.

Since the bi-realisation is supposed to be explicitly known, the construction of these terms can be done explicitly as well.

By construction, the Hamilton-Jacobi transform is the solution $S = \sum_{i=1}^{\infty} \frac{t^i}{i!} S_i \in \mathcal{C}^\infty(\mathcal{U})[[t]]$ of the *formal Hamilton-Jacobi equation*, which is a formal reformulation of equation (2.20) and is equivalent to (2.22):

$$\frac{\partial S_t}{\partial t} = \alpha^* H(dS_t) \text{ and } S_0 = 0$$

Step 2. Assume $S_t^{(k)} = \sum_{i=1}^{k} \frac{t^i}{i!} S_i$ is constructed. Now starts the construction of the Hamiltonian Poisson integrator itself. Choose a timestep, i.e. fix a small positive real number h. We define a numerical scheme approximating the integral curve of (2.21) with initial value x_0 by constructing the sequence $(x_n)_n$ according to the following recursion:

(a) Assume that for every $n \in \mathbb{N}$, the equation

$$\alpha\left(y_n, \sum_{i=1}^{k} h^i \nabla S_i(y_n))\right) = x_n$$

admits a unique solution y_n (otherwise, it means that the time step is too large).

(b) Set

$$x_{n+1} := \beta\left(y_n, \sum_{i=1}^{k} h^i \nabla S_i(y_n)\right).$$

Remark 2.4.2. The computations related to formal power series in Step 1. can be done efficiently with computer algebra tools[10]. Explicit formulae for (2.22) will be given with a systematic and combinatorial study in section 2.5.1. Let us give the first terms:

1. $S_1 = H$
2. $S_2 = \mathbf{0}^*\left(\{\alpha^* H, \tau^* S_1\}\right)$
3. $S_3 = \mathbf{0}^*\left(\{\alpha^* H, \tau^* S_2\} + \{\{\alpha^* H, \tau^* S_1\}, \tau^* S_1\}\right)$
4. $S_4 = \mathbf{0}^*\left(\{\alpha^* H, \tau^* S_3\} + 2\{\{\alpha^* H, \tau^* S_2\}, \tau^* S_1\} + \{\{\alpha^* H, \tau S_1\}, \tau^* S_2\} + \{\{\{\alpha^* H, \tau^* S_1\}, \tau^* S_1\}, \tau^* S_1\}\right).$

Above, the Poisson bracket is the one of the canonical symplectic form on $\mathcal{W}$ and $\mathbf{0}^*$ means that the function on $\mathcal{W}$ is restricted to $\mathcal{U} \times \{0\}$, therefore considered as a function on $\mathcal{U}$.

Remark 2.4.3. The resolution of the implicit relation in Step 2 can be done by approximation (for example by fixed point techniques) very efficiently: as any fixed point method, it can be done rapidly with given precision.

Mathematical details of the following important result can be found section 3.3.

Theorem 2.4.4. *The above numerical scheme defines a Hamiltonian Poisson integrator at order k for the Hamiltonian differential equation* (2.21).

Stated differently, for the Hamiltonian differential equation (2.21)*, given a bi-realisation $\mathcal{W}$ of $(\mathcal{U}, \pi)$, the diffeomorphism $\phi_h \colon \mathcal{U} \to \mathcal{U}$ associated to the bi-section given by the graph of the differential $\nabla S^{(k)} \sum_{i=1}^{k} \frac{t^i}{i!} \nabla S_i$, where $S_1, \ldots, S_k$ are the k-th first term of the formal Hamilton-Jacobi transform, is a Hamiltonian Poisson integrator of order k.*

Definition 2.4.5. We call this numerical scheme the k-th order Poisson integrator for H associated to the bi-realisation $\mathcal{W}$.

Example 2.4.6. For $k = 1$, this numerical scheme consists in mapping x_n to $\beta(y_n, h\nabla H(y_n))$ where y_n is the unique solution of $\alpha(y_n, h\nabla H(y_n)) = x_n$.

Example 2.4.7. In the case of a Lie-Poisson structure on a Lie algebra $\mathfrak{g}$ equipped with a local diffeomorphism $\varphi \colon G \to \mathfrak{g}$ with inverse $\psi \colon \mathfrak{g} \to G$, for $k = 1$, our Hamiltonian Poisson integrator of order 1 goes through the following steps:

[10] Some numerical methods of this thesis have been constructed using the Python library for symbolic mathematics SymPy.

1. Compute $a \mapsto (\psi(\eta))^{-1} T_\eta \psi(a)$, where $(\psi(\eta))^{-1}$ is the inverse of $\psi(\eta)$ for the group law of G, which is a family depending on $\eta \in \mathfrak{g}$ – η is close to zero in $\mathfrak{g}$ – of diffeomorphisms from $\mathfrak{g}$ to itself. Then consider the dual of its inverse, which is now a family of maps $D_\eta \colon \mathfrak{g}^* \simeq \mathfrak{g}^*$ being the identity map for $\eta = 0$. Then solve $D_{\Delta t \nabla H(y_n)}(y_n) = x_n$.

2. Consider
$$x_{n+1} = \mathrm{Ad}^*_{\psi(\Delta t \nabla y_n H)} x_n.$$

By construction, x_n and x_{n+1} belong to the same symplectic leaf.

Remark 2.4.8. At order $k = 1$ in the symplectic case (i.e. non-degenerate constant Poisson structure), it is easy to check that for the harmonic oscillator $H = \frac{p^2+q^2}{2}$, one recovers the symplectic mid-point scheme. For a general Hamiltonian H, the present construction gives the fact that an implicit Euler scheme of timestep $\frac{\Delta t}{2}$ composed with an explicit Euler scheme of timestep $\frac{\Delta t}{2}$ is a symplectic integrator of order at least 1 and timestep Δt. More generally, for higher orders the constructed Hamiltonian Poisson integrators for symplectic structures will be symplectic integrators, but they are in general different from the standard symplectic Runge-Kutta methods.

Remark 2.4.9. We have mentioned in the introduction that the naive idea "restrict to a leaf, be symplectic there" to recover Poisson globally, does not work because is almost never constructive. But the other way around it is actually fruitful: now having constructed a Hamiltonian Poisson integrator forcing the trajectory to stay on the correct leaf, one can apply the backward analysis techniques (restricted to leaves before globalizing) for error estimates, see section 4.2.

Remark 2.4.10. Recall that in the case of linear Poisson structures of Proposition 2.2.14, the construction of the bi-realisation amounts to computation of the coadjoint action of G on $\mathfrak{g}$, and construction of a local diffeomorphism: $\phi \colon G \to \mathfrak{g}$ with its differential at 1 being the identity.

The obtained Hamiltonian Poisson integrator of order 1 is of the form:

$$x_{n+1} = \mathrm{Ad}^*_{\phi^{-1}(\Delta t \nabla y_n H)} x_n$$

which is certainly not surprising: a symplectic leaf is an orbit of the coadjoint action and any such numerical scheme stays in the symplectic leaf where one starts from.

An obvious choice for ϕ is the inverse of the exponential map. As mentioned, there is some freedom in that choice: any such a local diffeomorphism can be used to compute a Hamiltonian Poisson integrator up to order k. It is important, however, to be able to compute easily its differential and its inverse.

It is remarkable that the point y_n where one computes the differential $\nabla_{y_n} H$ does not need to be in the coadjoint orbit of x_n. This shows that this method is deeply "Poisson in nature": we cannot simply restrict to a leaf and look for a symplectic integrator there: one has to look outside the symplectic leaf.

2.5 Algebra of Hamilton-Jacobi equation

2.5.1 The Farmer sequence and an algebraic formulae for the formal Hamilton-Jacobi equation

One sees from Equation (2.22) why the computation of first terms of the Taylor expansion with respect to t of the solution S_t of Hamilton-Jacobi equation, i.e. the formal Hamilton-Jacobi equation matters: if a bi-realisation can be constructed then each truncation at order k of this equation gives an explicit Hamiltonian Poisson integrator or order k as in Definition 2.4.5. We explain here some algebraic procedure that allows to compute recursively the terms of the formal series $S_t = \sum_{i=1}^{\infty} \frac{t^i}{i!} S_i$ that solves the formal Hamilton-Jacobi equation (2.22).

Let $\mathcal{P}_n$ be the list of all ordered tuples[11] $(p_1, \dots, p_k)$ of non-zero positive integers such that $p_1 + \cdots + p_k = n$, i.e. partitions of n. We warn the reader that, for us, $(1,3)$ and $(3,1)$ are different partitions of 4.

To any $(p_1, \dots, p_k) \in \mathcal{P}_n$, we now associate an integer $\beta(p_1, \dots, p_k)$ as follows. Define $\mathcal{S}$ as the free $\mathbb{N}$ module generated by polynomials with coefficients in $\mathbb{N}$. In short,

$$\mathcal{S} = \mathbb{N}\Big[\mathbb{N}[X]\Big].$$

We denote elements of $\mathcal{S}$ by $\sum_i n_i \diamond \left\{ P_i \right\}$ with $n_i \in \mathbb{N}$ and $P_i \in \mathbb{N}[X]$. Again, we warn the reader not to confuse $3 \diamond \left\{ 2X + X^2 \right\}$ with $\left\{ 6X + 3X^2 \right\}$: those are different elements in $\mathcal{S}$.

We now define a $\mathbb{N}$-linear endomorphism of $\mathcal{S}$ which is given for any polynomial $P \in \mathbb{N}[X]$ of degree $|P|$ by:

$$\begin{array}{rcl} I : \mathcal{S} & \longrightarrow & \mathcal{S} \\ P & \longmapsto & \sum_{i=1}^{|P|+1} \left\{ P + X^i \right\} \end{array}$$

Example 2.5.1. For instance $I\left(\left\{ X + X^2 \right\}\right) = \left\{ 2X + X^2 \right\} + \left\{ X + 2X^2 \right\} + \left\{ X + X^2 + X^3 \right\}$.

The following definition now makes sense:

Definition 2.5.2 (Farmer sequence)**.** Define the sequence $(\mathcal{A}_n)_{n \geqslant 1}$ valued in $\mathcal{S}$ as the iterations of I starting at $\left\{ X \right\}$:

$$\left\{ \begin{array}{rcl} \mathcal{A}_1 = & \left\{ X \right\} \\ \mathcal{A}_{n+1} = & I(\mathcal{A}_n) \end{array} \right. \tag{2.23}$$

Example 2.5.3. Let us give the first terms:

1. $\mathcal{A}_2 = \left\{ 2X \right\} + \left\{ X + X^2 \right\}$

[11] Our initial construction was quite different: the link with partitions is partially inspired by the work of Anton Fehnker, a master student at Göttingen Mathematisches Institut that was training for Mathematical Olympiads during Summer 2023.

2. $\mathcal{A}_3 = \left\{3X\right\} + 2 \diamond \left\{2X + X^2\right\} + \left\{X + 2X^2\right\} + \left\{X + X^2 + X^3\right\}$.

3. $\mathcal{A}_4 = \left\{4X, X + 3X^2\right\} + 3 \diamond \left\{2X + 2X^2\right\} + 3 \diamond \left\{3X + X^2\right\} + \left\{X + X^2 + 2X^3\right\} + 2 \diamond \left\{X + 2X^2 + X^3\right\} + 3 \diamond \left\{2X + X^2 + X^3\right\} + \left\{X + X^2 + X^3 + X^4\right\}$.

It is routine to check that $\mathcal{A}_n$ is a linear combination of polynomials P such that $P(1) = n$ and of the form $\sum_{i=1}^{k} p_i X^i$ where none of the integral coefficients $p_1, \ldots, p_k$ are zero. As a consequence,

$$\mathcal{A}_n = \sum_{(p_1,\ldots,p_k)\in\mathcal{P}_n} \beta(p_1, \ldots, p_k) \diamond \left\{p_1 X + \cdots + p_k X^k\right\}$$

for some integers $\beta(p_1, \ldots, p_k)$. Now, the following definition makes sense:

Definition 2.5.4. Let $(\mathcal{W}, \alpha, \beta)$ be a bi-realisation of $\mathcal{U}$ and let τ be the canonical projection $\tau : \mathcal{W} \to \mathcal{U}$. To any Hamiltonian $H \in \mathcal{C}^\infty(\mathcal{U})$, we associate a formal power series $S_H := \sum_{i=1}^{\infty} \frac{t^i}{i!} S_i$ in $\mathcal{C}^\infty(M)[[t]]$ where the sequence $(S_n)_{n\geqslant 1}$ is defined recursively by $S_1 = H$, and:

$$S_{n+1} = \sum_{(p_1,\ldots,p_k)\in\mathcal{P}_n} \beta(p_1, \ldots, p_k)\ \mathbf{0}^* \left(\mathrm{ad}_{\tau^* S_{p_k}} \ldots \mathrm{ad}_{\tau^* S_{p_1}} \alpha^* H\right).$$

where $\mathrm{ad}_g f = \{f, g\}$ is the adjoint action of the canonical Poisson bracket on $\mathcal{C}^\infty(\mathcal{W})$ and $\mathbf{0} \colon \mathcal{U} \to \mathcal{W}$ is the zero section of the vector bundle $\tau \colon T^*\mathcal{U} \to \mathcal{U}$.

Details of the following theorem are given section 3.3.4.

Theorem 2.5.5. *For any Hamiltonian function H on $(\mathcal{U}, \pi)$, and for any bi-realisation $(\mathcal{W}, \alpha, \beta)$ of $\mathcal{U}$, the formal function $S = \sum_{i=1}^{\infty} \frac{t^i}{i!} S_i \in \mathcal{C}^\infty(\mathcal{U})[[t]]$ is the solution of the formal Hamilton-Jacobi equation* (2.22) *(i.e. is the Hamilton-Jacobi transform of the Hamiltonian H) if and only if S verifies definition 2.5.4.*

Also, for every $k \geqslant 1$, the formal function $\sum_{i=1}^{k} \frac{t^i}{i!} S_i$ is a solution of the formal Hamilton-Jacobi equation up to order k.

As a consequence, we recover first terms of the formal Hamilton-Jacobi transform given in remark 2.4.2.

2.5.2 Magnus formula for the modified Hamiltonian

The definition of Hamiltonian Poisson integrator spots the importance of time-dependent Hamiltonians $(H_t)_t$ and of their Hamiltonian flow Φ_h. A main difference with classical Hamiltonians is that the existence of a first integral is not true anymore. This question is answered in this section in those terms: any non-autonomous (= time dependent) Hamiltonian flow admits a *formal Hamiltonian* which is also a *formal first integral*. See section 3.1 for details. The technique used in what follows relies on the construction of a Hamiltonian as a formal series $H\,[[\epsilon]] \in \mathcal{C}^\infty(M)\,[[\epsilon]]$ such that its time 1 flow is formally the time ϵ flow of $(H_t)_t$. There is an analogy with linear differential equations: the flow of

$$\dot{x}(t) = A \cdot x(t)$$

is given by the exponential $x(t) = e^{tA} \cdot x_0$. If the matrix A depends on t

$$\dot{x}(t) = A(t) \cdot x(t),$$

there exists a formal series $\tilde{A}[[\epsilon]]$ such that $x(\epsilon) = e^{\tilde{A}[[\epsilon]]} \cdot x_0$, see Magnus formula of [6]. We extend this formal series in the context of Poisson structures.

Definition 2.5.6. Let (H_t) be a time-dependent Hamiltonian function on $(\mathcal{U}, \pi)$. The Magnus formal series

$$\mathcal{M}_\epsilon(H) = \sum_{i=0}^{\infty} \frac{\epsilon^i}{i!} \mathcal{M}(H)_i \in \mathcal{C}^\infty(M)[[\epsilon]]$$

of $(H_t)_{t\in I}$ is defined by the formal differential equation:

$$\left\{ \begin{array}{ll} \mathcal{M}_0(H) & = 0 \\ \partial_\epsilon \mathcal{M}_\epsilon(H) & = \sum\limits_{i=0}^{\infty} \frac{B_i}{i!} \mathrm{ad}^i_{\mathcal{M}_\epsilon(H)} \sum_{j=0}^{\infty} \frac{\epsilon^j}{j!} \frac{\partial^j}{\partial t^j}\Big|_{t=0} H_t \end{array} \right. \tag{2.24}$$

where $\mathrm{ad}_{\mathcal{M}(H)} = \{\mathcal{M}(H), \cdot\}$, $\mathrm{ad}^i_{\mathcal{M}(H)}$ is the i-th power of the endomorphism $\mathrm{ad}_{\mathcal{M}(H)}$, and $\mathrm{ad}^0_{\mathcal{M}(H)} = Id$. Here, $(B_i)_{i\in\mathbb{N}}$ is the Bernoulli sequence, defined by its generating function: $\frac{x}{\exp(x)-1} = \sum\limits_{i=0}^{\infty} \frac{B_i}{i!} x^i$.

The terms of the Magnus formal series $\mathcal{M}(H)$ can be computed recursively out of equation (2.24), which ensures its existence and uniqueness.

Remark 2.5.7. There is another expression of the Magnus formal series obtained out of sucessive integration of (2.24), which results in the practical formula [6]:

$$\begin{array}{rcl} \mathcal{M}_\epsilon(H) & = & \int_0^\epsilon H_t \mathrm{dt} \\ & & -\frac{1}{2}\int_0^\epsilon \left\{ \int_0^{t_1} H_{t_2}\, \mathrm{dt}_2, H_{t_1} \right\} \mathrm{dt}_1 \\ & & +\frac{1}{6}\int_0^\epsilon \left\{ \int_0^{t_1} \left\{ \int_0^{t_2} H_{t_3}\, \mathrm{dt}_3, H_{t_2} \right\} \mathrm{dt}_2, H_{t_1} \right\} \mathrm{dt}_1 \\ & & + \dots \end{array} \tag{2.25}$$

For any $k \in \mathbb{N}$, we call *k-th Magnus truncation Hamiltonian*

$$\mathcal{M}_\epsilon(H)^{(k)} := \sum_{i=0}^{k} \frac{\epsilon^i}{i!} \mathcal{M}(H)_i$$

the sum of the $k+1$ first terms of the Magnus formal series $\mathcal{M}_\epsilon(H)$. By construction, for all given ϵ, $\mathcal{M}_\epsilon(H)^{(k)} \in \mathcal{C}^\infty(\mathcal{U})$ is a smooth Hamiltonian function on M for which we can speak about the Hamiltonian flow. The following theorem, proved in section 3.1, aims at approximating a non-autonomous Hamiltonian flow by an autonomous one at any order.

Theorem 2.5.8. *Let $(H_t)_{t\in I}$ be a time-dependent Hamiltonian for the Poisson structure $(\mathcal{U}, \pi)$. For any $k \in \mathbb{N}$:*

- *the flow $\Phi^\epsilon_{(H_t)_t}$, at time ϵ, of the time-dependent Hamiltonian $(H_t)_{t\in I} \in \mathcal{C}^\infty(\mathcal{U} \times I)$,*
- *and the flow $\Phi^1_{\mathcal{M}_\epsilon(H)^{(k)}}$, at time 1, of the k-th Magnus truncation Hamiltonian $\mathcal{M}_\epsilon(H)^{(k)} \in \mathcal{C}^\infty(M)$,*

coincide up to order k in ϵ.

Remark 2.5.9. Theorem 2.5.8 can be restated in terms of the local coordinates $x_1, \dots, x_n$:

$$\forall\, 0 \leqslant j \leqslant k, \quad \left.\frac{\partial^j}{\partial \epsilon^j}\right|_{\epsilon=0} \Phi^{\epsilon}_{(H_t)_t}(x) = \left.\frac{\partial^j}{\partial \epsilon^j}\right|_{\epsilon=0} \Phi^{1}_{\mathcal{M}_\epsilon(H)^{(k)}}(x). \tag{2.26}$$

It is therefore an equality of the k-th first jets of the integral curve for the time-dependent Hamiltonian functions $(H_t)_t$ and the integral curve for the Hamiltonian $\mathcal{M}_\epsilon(H)^{(k)}$.

We apply now theorem 2.5.8 to Hamiltonian Poisson integrators that have been constructed above. To do so, we use the following formula:

Proposition 2.5.10. *Consider a Hamiltonian Poisson integrator ϕ^k_ϵ as in Definition 2.4.5. Let $(S^{(k)}_\epsilon)_\epsilon$ be the solution at order k of the formal Hamilton-Jacobi equation* (2.20)*. A time-dependent Hamiltonian $(H^k_t)_t$ for ϕ^k_ϵ is given for all $x \in \mathcal{U}$, by*

$$H^k_t(x) = \frac{dS^{(k)}_t}{dt}(y)$$

where y is the solution of $\alpha(y, \nabla \frac{dS^{(k)}_t}{dt}(y)) = x$.

Remark 2.5.11. Let us spell out H^k_t using a bi-realisation $\mathcal{W}$ on the open subset $\mathcal{U}$.

$$H^k_t = \frac{\mathrm{d}S^k_t}{\mathrm{d}t} \circ \tau_{|L^k_t} \circ \alpha^{-1}_{|L^k_t} \tag{2.27}$$

where $\tau \colon T^*M \to M$ is the cotangent projection and L^k_t is the bi-section given by the graph of $\mathrm{d}S^k_t$.

The previous statements altogether give the concluding corollary of this section by applying the Magnus formula to the time-dependent Hamiltonian H^k_t obtained from S^k_t through Proposition 2.5.10.

Corollary 2.5.12. *1. Any Hamiltonian Poisson integrator admits a formal modified Hamiltonian: obtained by applying the Magnus formula to the time-dependent Hamiltonian $(H_t)_{t\in I}$.*

2. Moreover, in the case of the k-th order Hamiltonian Poisson integrator constructed out of a bi-realisation as in Definition 2.4.5, this modified Hamiltonian $\mathcal{M}_\epsilon((H^k_t)_t)$ coincides with ϵH up to order k: $\mathcal{M}_\epsilon((H^k_t)_t) = \epsilon H + o\big(\epsilon^k\big)$.

In particular, truncating $\mathcal{M}_\epsilon((H^k_t)_t)$ at any finite order in ϵ, we get a smooth first integral up to the order of truncation. Similar techniques have been used in [5] to explain the good behaviour of symplectic integrators on long run simulations.

2.6 Numerical behaviour of Hamiltonian Poisson integrator

This section introduces section 4.2 and sums up numerical properties of our Hamiltonian Poisson integrators. Consider the Hamiltonian Poisson integrator $\varphi^k_{\Delta t}$ of Hamiltonian H, order k and time-step Δt associated to an explicit bi-realisation $\mathcal{W}$ of $(\mathcal{U}, \pi)$ as in Definition 2.4.5.

Properties of one iteration: symplectic leaves are preserved By definition of the order, the norm of the difference between the trajectory $\Phi_H^{\Delta t}(x)$ we are looking for and its approximation $\varphi_{\Delta t}^k(x)$ is controlled by $(\Delta t)^k$:

$$\|\varphi_{\Delta t}^k(x) - \Phi_{\Delta t}^H(x)\| \leqslant C(\Delta t)^k \tag{2.28}$$

for some constant $C > 0$, at least on a relatively compact open subset.

Now, for every x in $\mathcal{U}$, x and $\varphi_{\Delta t}^k(x)$ (provided that the second is well-defined) are in the same symplectic leaf up to the precision of which one is able to solve the nonlinear equation in y

$$\alpha(y, \nabla S_{\Delta t}^{(k)}(y)) = x. \tag{2.29}$$

This precision a priori only depends on the nonlinear solver we use. However, in general, since it can be solved with a fixed point method, it can be solved with "machine precision" using only few computations.

Last, the Hamiltonian function H is not preserved by our Hamiltonian Poisson integrator. However, the formal modified Hamiltonians $H_{\Delta t}$ does satisfy

$$H_{\Delta t}(\phi_{\Delta t}^k(x)) = H_{\Delta t}(x).$$

Properties of the discrete trajectory For any k-th order numerical integrator, if we repeat the operation N times, the distance between the discrete solution given by the integrator and the real solution of the differential equation may grow linearly in $N(\Delta t)^k$. However, since symplectic leaves are preserved with given precision, we can expect that the discrete trajectory will preserve Casimir in an excellent way. Moreover, provided that the formal modified Hamiltonian H_ϵ is not just a formal function but a real function, it will be constant along the discrete trajectories of the integrator. Since $\frac{1}{\epsilon}H_\epsilon$ and H coincide up to order $(\epsilon)^k$, it implies that the Hamiltonian function H itself is going to be relatively well preserved. In our numerical examples (see chapter 4), oscillations around the level $H^{-1}(\{H(x)\})$ of H are observed: their amplitude is controlled by the order of the method. The simultaneous control on the distance to the symplectic leaf and on the distance to an energy level for a generic Hamiltonian is of course a very important feature explaining this good long-term behaviour.

Preservation of symmetries will also be illustrated on the rigid body dynamic example, see section 4.2.1. As we will see, the most interesting discrete dynamics happens on long-run simulations.

Another remarkable fact is the stability in a neighborhood of a singularity: along an exploding trajectory, a Hamiltonian Poisson integrator sticks to the continuous trajectory much longer than a traditional method. This phenomenon is illustrated on a Lotka-Volterra system, see section 4.2.2.

Up to here, we have used words such as "stability", "exploding" and "symmetries" without definition. We will illustrate them in chapter 4.

CHAPTER 3

Symplectic groupoids for Poisson integrators

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Introduction

In this self-consistent chapter, we address the question of Hamiltonian Poisson integrators in a more systematic manner than in the overview in chapter 2: we will now from scratch consider generic Poisson manifolds by using the concept of symplectic Lie groupoids, and, of course, we will prove prove the theorems presented in chapter 2.

Recall that Poisson integrators are examples of so-called geometric integrators, which are numerical methods for solving differential equations, designed to preserve some geometric structure naturally associated to the studied system. The first and the best studied geometric numerical methods are symplectic integrators, also called symplectic schemes[1]. Symplectic integrators (see e.g. [75]) are suited to discretize the flow of Hamiltonian equations, and as their name suggests, are designed to preserve the symplectic structure in the process. Qualitatively, this results in a better control on the conservation of the energy of the system ([59]), even for simulations on large time intervals. Designed in the early eighties, they are now widely used in various applications, like conservative large scale molecular dynamics [70]. Some work followed and attempted to preserve various structures naturally associated to the phase space of the system or to the system itself; detailed literature review can be found in [32] and references therein for integrators preserving several structures from classical differential geometry, and in a more recent review [63] for structures coming from more contemporary "higher" and "generalized" geometry.

Poisson geometry permits to generalize simultaneously Hamiltonian mechanics on symplectic manifolds and Lie group dynamics. Furthermore, it is an efficient tool to study symmetries of a large class of dynamical systems, arising from conservative equations such as the ones of celestial mechanics [2], rigid body [47], Toda lattices [4], Korteweg-de-Vries equation [1], Lotka-Volterra systems [41], to cite a few. Except for the first one, those are associated to non-symplectic Poisson structures. A natural question is then the design of numerical methods that take into account this geometry in order to find reliable approximations of solutions. And this question was indeed addressed right after the appearance of symplectic integrators. The first of them were based on an important result that a Poisson manifold is foliated into symplectic leaves [10], the idea being essentially that the dynamics shoud be restricted to a leaf, so that a usual symplectic integrator can be used. The main issue of this approach is that having a Poisson structure where one can explicitly (and globally) describe the leaves is a very strong assumption, so the class of systems where the construction applies is rather small. The next class of papers ([26], [56]) made a step forward in this direction, enforcing the condition of preservation of the leaves of the Poisson foliations, being often not explicit but conceptually more appropriate. However, we have observed (see Example 3.2.24) that some of these constructions applied naively do not produce the desired results in terms of energy conservation. More recently, the authors [23] have constructed Poisson integrators for dual of Lie algebroids (i.e. fiberwise linear Poisson structures on a vector bundle), understood them through Hamilton-Jacobi equations and Lagrangian bi-sections (see also [26]). These are elements that appear in the present study as well, but now for generic Poisson structures.

Indeed, in this chapter, we revisit and explain the above mentioned problems in the more conceptual and general framework of manifolds and differential geometry. We introduce a (stronger) notion of a Hamiltonian Poisson integrator, which takes into account simultaneously the geometry of the phase

[1]Throughout this chapter we will use "integrators", "schemes" and "numerical methods" as synonyms.

space (Poisson structure) and the physics of the system (Hamiltonian function). Moreover we make this idea constructive by using the local symplectic groupoid associated to Poisson manifolds. Since the symplectic groupoid inducing this Poisson structure on its unit can be thought of as a bigger foliated space where the foliation has been desingularized, the discretized dynamics we suggest uses heavily the idea to lift the picture to this groupoid and project back at each time step – with an explicit construction.

The chapter is organized as follows. In sections 1 and 2, we introduce the necessary mathematical background for the construction of Hamiltonian Poisson integrators. First, we adapt the Magnus formula to time-dependent Hamiltonian systems. Second, we explain the concept of families of Lagrangian bi-sections of symplectic groupoids. This is already enough to formulate the notion of Hamiltonian Poisson integrators and give several properties, like, e.g. backward analysis. Then in section 3, we use Hamilton-Jacobi equation to make this idea constructive, namely to produce smooth families of Lagrangian bi-sections inducing Poisson integrators that approximate at any given order the Hamiltonian flow.

In the sequel, (M, π) is a Poisson manifold, whose Poisson bracket will be denoted by $\{F, G\}$ for all $F, G \in \mathcal{C}^\infty(M)$. Also, $\epsilon \in I \subset \mathbb{R}$ is a real number (thought of as being small and positive when having numerical applications in mind), called *discretization parameter*.

Below is a list of references for several notions that we will not recall:

1. Poisson manifolds $(M, \pi = \{\cdot, \cdot\})$, [43, 18]. The Poisson structure will be denoted by π when considered as a section of $\Lambda^2 TM$ or by $(F, G) \mapsto \{F, G\}$ when considered as biderivation of smooth functions.

2. Lie groupoids and local Lie groupoids [51, 16], denoted respectively as $\mathcal{G} \rightrightarrows M$ and $\mathfrak{U}(M) \rightrightarrows M$. For all considered local or global groupoids, the source shall be denoted by α and the target by β.

3.1 Hamiltonian Magnus formula

For $A(t)$ a time-dependent linear operator, the Magnus formula allows to make the time ϵ flow of a time-dependent linear differential equation $\dot{x} = A(t)x$ of order 1 as an exponential $x(\epsilon) = \exp(B_\epsilon)x(0)$. In general, there are convergence issues that forbid B_ϵ to be defined out of $A(t)$ for a given value of ϵ, but it is well-defined as a formal series in ϵ. More generally, the Magnus formula allows to express, up to convergence issues, the flow at a given time ϵ of a time-dependent left-invariant vector field on a Lie group by an exponential trajectory at time 1 of a left invariant vector field depending on ϵ (but not depending on the time t). A review on Magnus expansion can be found in [6]. The aim of the present section is to adapt the idea to time-dependent Hamiltonian differential equations on a Poisson manifold.

A *time-dependent function* on a manifold M is a family $(H_t)_{t\in I}$ of functions on M that depend smoothly on the parameter t – living in an open interval I containing 0 – in the sense that $(m, t) \mapsto H_t(m) \in \mathcal{C}^\infty(M \times I)$. For (M, π) a Poisson manifold, a time-dependent function $(H_t)_{t\in I} \in \mathcal{C}^\infty(M \times I)$ will be referred to as a *time-dependent Hamiltonian function*. It induces a time-dependent vector field $X_{H_t} := \{H_t, \cdot\}$ called *time-dependent Hamiltonian vector field*.

We call *formal Taylor expansion* of $(H_t)_{t\in I}$ the formal series

$$H\left[[\epsilon]\right] := \sum_{i\geqslant 0} \frac{\epsilon^i}{i!} \left.\frac{\partial^i H_t}{\partial t^i}\right|_{t=0} \in \mathcal{C}^\infty(M)\left[[\epsilon]\right].$$

One must not confuse the formal Taylor expansion of a Hamiltonian function $(H_t)_{t\in I}$ (which does not depend on the Poisson structure π) with a second and more subtle formal series in $\mathcal{C}^\infty(M)\left[[\epsilon]\right]$ defined as follows:

Definition 3.1.1. The Magnus formal series

$$\mathcal{M}_\epsilon(H) = \sum_{i=0}^{\infty} \frac{\epsilon^i}{i!} \mathcal{M}(H)_i \in \mathcal{C}^\infty(M)\left[[\epsilon]\right]$$

of $(H_t)_{t\in I}$ is defined by the formal differential equation:

$$\left\{ \begin{array}{ll} \mathcal{M}_0(H) & = 0 \\ \partial_\epsilon \mathcal{M}_\epsilon(H) & = \sum\limits_{i=0}^{\infty} \frac{B_i}{i!} \mathrm{ad}^i_{\mathcal{M}_\epsilon(H)} \Big(H\left[[\epsilon]\right]\Big) \end{array} \right. \tag{3.1}$$

where $\mathrm{ad}^i_{\mathcal{M}_\epsilon(H)}$ is the i-th power of the endomorphism $\mathrm{ad}_{\mathcal{M}_\epsilon(H)} = \{\,\mathcal{M}_\epsilon(H), \cdot\,\}$, and $\mathrm{ad}^0_{\mathcal{M}(H)} = Id$. Also, $(B_i)_{i\in\mathbb{N}}$ is the Bernoulli sequence, defined by its generating function: $\frac{x}{\exp(x)-1} = \sum\limits_{i=0}^{\infty} \frac{B_i}{i!} x^i$.

The terms of the Magnus formal series $\mathcal{M}(H)\left[[\epsilon]\right]$ can be computed recursively out of equation (3.1), which ensures its existence and uniqueness.

Remark 3.1.2. There is another expression of the Magnus formal series obtained out of sucessive integration of (3.1), which results in the practical formula [6]:

$$\begin{array}{rcl} \mathcal{M}_\epsilon(H) & = & \int_0^\epsilon H_t \mathrm{dt} \\ & & -\frac{1}{2}\int_0^\epsilon \Big\{ \int_0^{t_1} H_{t_2}\,\mathrm{dt}_2, H_{t_1} \Big\}\,\mathrm{dt}_1 \\ & & +\frac{1}{6}\int_0^\epsilon \Big\{ \int_0^{t_1} \Big\{ \int_0^{t_2} H_{t_3}\,\mathrm{dt}_3, H_{t_2} \Big\}\,\mathrm{dt}_2, H_{t_1} \Big\}\,\mathrm{dt}_1 \\ & & +\dots \end{array} \tag{3.2}$$

Let us explain the meaning of this expression. Assume we wish to compute the third term $\frac{\epsilon^3}{3!}\mathcal{M}(H)_3$ in the Magnus formal series. For that purpose, it suffices to find the term in ϵ^3 in each one of the first two terms of (3.2):

$$\begin{array}{rcl} \int_0^\epsilon H_t \mathrm{dt} & = & \epsilon H_0 + \frac{\epsilon^2}{2} \left.\frac{\partial H_t}{\partial t}\right|_{t=0} + \frac{\epsilon^3}{6} \left.\frac{\partial^2 H_t}{\partial t^2}\right|_{t=0} + \cdots \\ \int_0^\epsilon \Big\{ \int_0^{t_1} H_{t_2}\,\mathrm{dt}_2, H_{t_1} \Big\}\,\mathrm{dt}_1 & = & \frac{\epsilon^3}{6}\{H_0, \left.\frac{\partial H_t}{\partial t}\right|_{t=0}\} + \cdots \end{array} \tag{3.3}$$

and to add them up.

Example 3.1.3. For a time-independent Hamiltonian $(H_t)_{t\in I}$ with $H_t = H$ for all $t \in I$, the Magnus formal series is ϵH.

Example 3.1.4. If M and N are two Poisson manifolds, $\phi\colon M \to N$ is a Poisson map and $(H_t)_{t\in I}$ is a time-dependent Hamiltonian on N: $\mathcal{M}_\epsilon(\phi^* H) = \phi^* \mathcal{M}_\epsilon(H)$.

For any $k \in \mathbb{N}$, we call *k-th Magnus truncation Hamiltonian* and we denote by

$$\mathcal{M}_\epsilon(H)^{(k)} := \sum_{i=0}^{k} \frac{\epsilon^i}{i!} \mathcal{M}(H)_i$$

the sum of the $k+1$ first terms of the Magnus formal series $\mathcal{M}_\epsilon(H)$. By construction, for all given ϵ, $\mathcal{M}_\epsilon(H)^{(k)} \in \mathcal{C}^\infty(M)$ is a smooth Hamiltonian function on M.

Theorem 3.1.5. *Let $(H_t)_{t\in I}$ be a time-dependent Hamiltonian on a Poisson manifold (M,π). For any $k \in \mathbb{N}$:*

(i) the flow $\Phi^\epsilon_{(H_t)_t}$, at time ϵ, of the time-dependent Hamiltonian $(H_t)_{t\in I} \in \mathcal{C}^\infty(M \times I)$,

(ii) and the flow $\Phi^1_{\mathcal{M}_\epsilon(H)^{(k)}}$, at time 1, of the k-th Magnus truncation Hamiltonian $\mathcal{M}_\epsilon(H)^{(k)} \in \mathcal{C}^\infty(M)$,

coincide up to order k in ϵ.

In other words, for all $f \in \mathcal{C}^\infty(M)$ and $0 \leqslant j \leqslant k$:

$$\left.\frac{\partial^j}{\partial \epsilon^j}\right|_{\epsilon=0} \left(\Phi^\epsilon_{(H_t)_t} - \Phi^1_{\mathcal{M}_\epsilon(H)^{(k)}}\right)^* f \;=\; 0. \tag{3.4}$$

Proof. The computation is a formal Hamiltonian analog of [6].

Set $f_\epsilon^{(k)} \in \mathcal{C}^\infty(M)[[\epsilon]]$ the formal Taylor expansion of ${\Phi^1_{\mathcal{M}_\epsilon(H)^{(k)}}}^* f$, where pull-backs of smooth maps are defined on formal series in an obvious way. The definition of $\mathcal{M}(H)$ implies the following equalities of formal series :

$$\partial_\epsilon(f_\epsilon^{(k)}) = {\Phi^1_{\mathcal{M}_\epsilon(H)^{(k)}}}^* \sum_{i=0}^{\infty} \frac{1}{(i+1)!} \mathrm{ad}^i_{X_{\mathcal{M}_\epsilon(H)^{(k)}}} . \partial_\epsilon X_{\mathcal{M}_\epsilon(H)^{(k)}}(f) \tag{3.5}$$

$$= {\Phi^1_{\mathcal{M}_\epsilon(H)^{(k)}}}^* \sum_{i=0}^{\infty} \frac{1}{(i+1)!} \mathrm{ad}^i_{X_{\mathcal{M}_\epsilon(H)^{(k)}}} . \sum_{j=0}^{k-1} \frac{B_j}{j!} \mathrm{ad}^j_{X_{\mathcal{M}_\epsilon(H)^{(k)}}} . X_{H_\epsilon}(f) + o\left(\epsilon^{k-1}\right). \tag{3.6}$$

The definition of Bernoulli numbers and the equality $\sum_{i\in\mathbb{N}} \frac{x^i}{(i+1)!} = \frac{\exp x - 1}{x}$ implies the simplification

$$\partial_\epsilon(f_\epsilon^{(k)}) = {\Phi^1_{\mathcal{M}_\epsilon(H)^{(k)}}}^* X_{H_\epsilon}(f) + o\left(\epsilon^{k-1}\right). \tag{3.7}$$

As $\Phi^0_{(H_t)_t} = \Phi^1_{\mathcal{M}_0(H)^{(k)}} = \mathrm{Id}$, the result follows by differentiation. □

Remark 3.1.6. Theorem 3.1.5 can be restated using functions of particular interest in mechanics, namely local coordinates x on M:

$$\forall\, 0 \leqslant j \leqslant k, \quad \frac{\partial^j}{\partial \epsilon^j}\Big|_{\epsilon=0} (\Phi^\epsilon_{(H_t)_t} - \Phi^1_{\mathcal{M}_\epsilon(H)^{(k)}})(x) = 0, \tag{3.8}$$

so that both integral curves at x coincide up to order k.

Remark 3.1.7. A particular case of the Magnus formula in the symplectic setting appears in [39], Section 19, where the author studies symplectic integrators for the harmonic oscillator. Up to different conventions, Equation (19.9) is the Magnus formula of the Hamiltonian of Equation (19.11).

Several time-dependent Hamiltonian vector fields we dealt with in this section arise while studying geometric integrators of Hamiltonian systems that do not depend on time. Indeed, under some general assumptions, each iteration of a Poisson integrator for a Hamiltonian H is the time ϵ-flow of a time-dependent Hamiltonian (H_t), as will be detailed in 3.2.4. To have an integrator at order k, we will require the Magnus series $\mathcal{M}_\epsilon((H_t)_t)$ of (H_t) to coincide with ϵH at order k.

3.2 Hamiltonian Poisson integrators

In order to define and study Poisson integrators, we recall simple facts of symplectic geometry.

3.2.1 Smooth families of Lagrangian submanifolds

Definition 3.2.1. Let V be a manifold. A family $(L_t)_{t\in I}$ of submanifolds of V parametrized by I is said to be a *smooth family of submanifolds* of V if $L_I = \{(x,t) \in V \times I, x \in L_t\}$ is a submanifold of $V \times I$ such that the restriction to L_I of the projection $V \times I \to I$ is a surjective submersion.

From now on, we fix $(L_t)_{t\in I}$ a smooth family of submanifolds of V, and $L_I \subset V \times I$ as in Definition 3.2.1. Let $t_0 \in I$ and $NL_{t_0} = TV|_{L_{t_0}}/TL_{t_0}$ be the normal bundle of L_{t_0}. We claim that there is a canonically defined smooth section

$$\left[\frac{\partial L_{t_0}}{\partial t_0}\right] \in \Gamma(NL_{t_0})$$

called the *normal variation of* $(L_t)_{t\in I}$ *at* t_0. We begin with a definition.

Definition 3.2.2. A smooth path $\gamma\colon I \to V$ is said to be an $(L_t)_{t\in I}$-path if $\gamma(s) \in L_s$ for all $s \in I$. Equivalently, an $(L_t)_{t\in I}$-path is a smooth path $\gamma\colon I \to V$ such that $s \mapsto (\gamma(s), s)$ is valued in the submanifold $L_I \subset V \times I$.

The existence, uniqueness and smoothness of the normal variation follow from the three items of Lemma 3.2.3 respectively.

Lemma 3.2.3. *Let $(L_t)_{t\in I}$ be as above.*

1. *Let $t_0 \in I$ and $x \in L_{t_0}$. There exists at least one $(L_t)_{t\in I}$-path γ, defined in an open neighborhood of t_0, such that $\gamma(t_0) = x$.*
2. *For any two paths γ_1, γ_2 as in the first item, $\dot\gamma_1(t_0) - \dot\gamma_2(t_0) \in T_xL_{t_0}$.*
3. *The map assigning to $x \in L_{t_0}$ the class in the normal bundle of the derivative $\dot\gamma(t_0)$ of a path as in the first item is a smooth section of the normal bundle.*

Proof. The I-valued path $t \mapsto t$ lifts through $L_I \twoheadrightarrow I$ to a path γ with $\gamma(t_0) = (x, t_0)$, because the latter map is a surjective submersion by assumption. The two remaining items are straightforward and left to the reader. □

From now on, let us assume that V is equipped with a symplectic 2-form ω_V. A smooth family of submanifolds $(L_t)_{t\in I}$ is said to be *a smooth family of Lagrangian submanifolds* when all the submanifolds L_t are Lagrangian. Under these assumptions, for all $t \in I$, the normal bundle TV/TL_t is canonically isomorphic to T^*L_t and the normal variation is a family of 1-forms $\xi_t \in \Omega^1(L_t)$, called *variation form of* $(L_t)_{t\in I}$ *at* t. In equation:

$$\omega_V\left(\left[\tfrac{\partial L_t}{\partial t}(x)\right]\Big|_t, u\right) = \xi_t(u) \text{ for all } u \in T_xL_t \tag{3.9}$$

The following lemma is left to the reader as well:

Lemma 3.2.4. *Let $(L_t)_{t\in I}$ be a smooth family of Lagrangian submanifolds. The variation form $\xi_t \in \Omega^1(L_t)$ of $(L_t)_{t\in I}$ at $t \in I$ is a closed 1-form.*

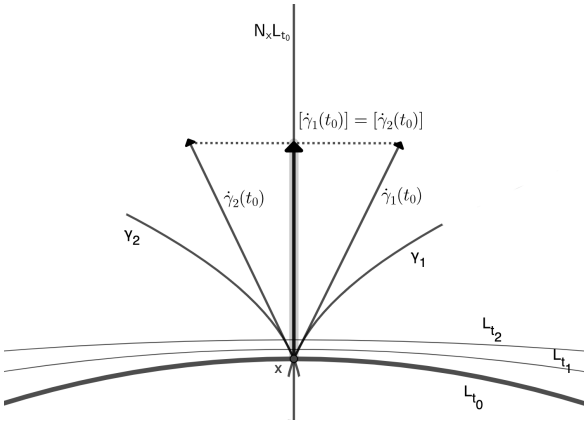


Figure 3.1: Normal variation of L_{t_0} at x out of two L-paths γ_1 and γ_2.

Definition 3.2.5. We call *exact* a smooth family of Lagrangian submanifolds $(L_t)_{t\in I}$ such that its corresponding variation 1-forms $(\xi_t)_{t\in I}$ are exact; we call *variation functions* their primitives, i.e. some time-dependent functions $(h_t)_{t\in I}$ such that $dh_t = \xi_t$ for all $t \in I$.

Remark 3.2.6. For a given smooth family of *exact* Lagrangian submanifolds, the family of time-dependent functions $(h_t)_{t\in I}$ is unique up to a time-dependent constant.

Here are two important classes of smooth families of Lagrangian submanifolds.

Example 3.2.7. Let V be a symplectic manifold, and $H \in C^\infty(V)$ a Hamiltonian function whose Hamiltonian vector field admits a flow for all $t \in \mathbb{R}$. For every Lagrangian submanifold $L \subset V$, the family $L_t = \phi_H^t(L)$ is an exact smooth family of Lagrangian submanifolds. An L-path starting at $x \in L$ is given by the flow $(\phi_H^t(x))_t$ of H and the variation form of L at t is the restriction to L_t of the exact form dH.

Example 3.2.8. Let T^*Q be a cotangent bundle. For every smooth family of closed one-forms $(\zeta_t)_{t\in I}$ on Q, their graphs $L_t = \bar{\zeta_t} = \{\zeta_t(x), x \in Q\}$ form a smooth family of Lagrangian submanifolds. An L-path starting at $x \in \bar{\zeta_0}$ is given by the 1-forms $(\zeta_t(x))_t$ and the variation form at t is $\tau^*_{|\bar{\zeta_t}}\partial_t\zeta_t$, where $\tau\colon T^*Q \to Q$ is the cotangent projection and $\tau_{|\bar{\zeta_t}}\colon \bar{\zeta_t} \xrightarrow{\sim} Q$ its restriction to $\bar{\zeta_t}$.

Variation forms behave well with respect to symplectomorphisms, as explained in the following example.

Example 3.2.9. Let (V, ω_V) and (W, ω_W) be two symplectic manifolds, $\phi\colon V \xrightarrow{\sim} W$ a bijective symplectomorphism and $(L_t)_t$ a smooth family of Lagrangian submanifolds with variation 1-forms ξ_t. Then, $\tilde{L}_t = \phi(L_t)$ is also a smooth family of Lagrangian submanifolds with variation 1-forms $\tilde{\xi}_t$ that verify $\phi^*\tilde{\xi}_t = \xi_t$.

3.2.2 Usual Hamilton-Jacobi equation revisited

This section is independent from the core of the chapter but we think it matters for terminology and pedagogical interest. We use variation forms to reinterpret the usual Hamilton-Jacobi equation in terms of smooth families of Lagrangian submanifolds. Consider a Hamiltonian $H \in \mathcal{C}^\infty(T^*Q)$ on the cotangent bundle T^*Q of a manifold Q. The Hamilton-Jacobi equation consists in looking for a family

of functions $S_t \in C^\infty(Q \times Q)$, depending smoothly on t in some interval $I \subset \mathbb{R}$, such that for every $(q, \bar{q}) \in Q \times Q$ and every $t \in I$:

$$\partial_t S_t(q, \bar{q}) = H(\mathrm{d}_q S_t(q, \bar{q})) \tag{3.10}$$

where $\mathrm{d}_q S_t(q, \bar{q}) \in T_q^* Q$ is the differential of $S(\cdot, \bar{q})$ at the point q, so that $(q, \bar{q}) \mapsto H(\mathrm{d}_q S_t(q, \bar{q})) \in C^\infty(Q \times Q)$.

Theorem 3.2.10 (Hamilton-Jacobi theorem for a cotangent bundle)**.** *If $(S_t)_{t\in I}$ verifies equation (3.10), if there exist open subsets $\mathcal{U} \subset Q \times Q$ and $\mathcal{V} \subset T^*Q$ between which $(q, \bar{q}) \mapsto d_q S_t(q, \bar{q})$ is a diffeomorphism for every $t \in I$ and if their exists $\epsilon_0 \in J$ such that the Hamiltonian flow $\Phi_H^{\epsilon_0}$ of $H \in \mathcal{C}^\infty(T^*Q)$ at time ϵ_0 is given by:*

$$\Phi_H^{\epsilon_0}(\zeta) = d_{\bar{q}} S_{\epsilon_0}(q, \bar{q}) \qquad \forall \zeta \in \mathcal{V} \subset T^*Q \tag{3.11}$$

where $(q, \bar{q}) \in Q \times Q$ is the unique element in $\mathcal{U}$ that satisfies $\zeta = -d_q S_{\epsilon_0}(q, \bar{q})$, then the Hamiltonian flow Φ_H^ϵ of $H \in \mathcal{C}^\infty(T^*Q)$ at time $\epsilon \in I$ is given by:

$$\Phi_H^{\epsilon}(\zeta) = d_{\bar{q}} S_{\epsilon}(q, \bar{q}) \qquad \forall \zeta \in \mathcal{V} \subset T^*Q. \tag{3.12}$$

Classical literature [54] defines elements in T^*Q as pairs (q, p) with $q \in Q$ and $p \in T_q^*Q$, and the map $\Phi_\epsilon^H : (q, p) \mapsto (\bar{q}, \bar{p})$ above is then seen as being implicitly defined by:

$$\begin{cases} \bar{q} &= \partial_q S_\epsilon(q, \bar{q}) \\ \bar{p} &= -\partial_{\bar{q}} S_\epsilon(q, \bar{q}) \end{cases} \tag{3.13}$$

Let us use the tools developed in subsection 3.2.1 to give an interpretation and a proof of Theorem 3.2.10.

Proof. Geometrically, two families of Lagrangian submanifolds are involved here:

1. Since $\Phi_H^t : T^*Q \to T^*Q$ is a symplectomorphism, its graph $\underline{\Phi_H^t} = \{(x, \Phi_H^t(x)) \in T^*Q \times T^*Q,\ x \in T^*Q\}$, is a Lagrangian submanifold of $T^*Q \times T^*Q$ equipped with the product symplectic form with positive and negative signs on first and second factor respectively. As in example 3.2.7, variation forms of $(\underline{\Phi_H^t})_t$ are $(\xi_t)_t = (\Phi_H^{-t *} \mathrm{d}H)_t$, where Φ_H^{-t} is understood as a map $\Phi_H^{-t} : \underline{\Phi_H^t} \to T^*Q$.

2. For every $t \in J$, the graph of the exact form $\underline{\mathrm{d}S_t}$ is a Lagrangian submanifold of $T^*(Q \times Q)$ equipped with its canonical symplectic form. As in example 3.2.8, variation forms of $(\underline{\mathrm{d}S_t})_t$ are $(\tilde{\xi}_t)_t = (\tau^*_{|\mathrm{d}S_t} \mathrm{d}\frac{\partial}{\partial_t} S_t)_t$, for τ the cotangent projection.

Now, the two symplectic manifolds above are canonically symplectomorphic:

$$\begin{array}{rccc} \Psi : & T^*Q \times T^*Q & \to & T^*(Q \times Q) \\ & (\zeta(q), \bar{\zeta}(\bar{q})) & \mapsto & \zeta(q) - \bar{\zeta}(\bar{q}) \end{array} . \tag{3.14}$$

As in 3.2.9, both variation forms are related by Ψ, hence:

$$\mathrm{d}\partial_t S_t = (\Phi_H^{-t} \Psi^{-1} \tau^{-1}_{|\mathrm{d}S_t})^* \mathrm{d}H. \tag{3.15}$$

Since Φ_H^{-t} restricted to $\Psi^{-1}\tau^{-1}_{|\mathrm{d}S_t}(Q \times Q)$ corresponds with the projection on first factor of $T^*Q \times T^*Q$, for any $(q, \bar{q}) \in Q \times Q$,

$$\Phi_H^{-t} \Psi^{-1} \tau^{-1}_{|\mathrm{d}S_t}(q\bar{q}) = \mathrm{d}S_t(q, \bar{q}) \tag{3.16}$$

and the equation

$$\mathrm{d}\partial_t S_t(q,\bar{q}) = \mathrm{d}(\mathrm{d}_q S_t)^* H \tag{3.17}$$

follows. It is clear that a time-dependent constant can be added to generating functions $(S_t)_t$. Equation (3.17) is Hamilton-Jacobi equation (3.10) up to a time-dependent coboundary. This completes the proof of theorem 3.2.10. □

As a conclusion, one geometric interpretation of Hamilton-Jacobi equation is that the canonical symplectomorphism (3.14) above intertwines the two families of Lagrangian submanifolds $(\underline{\mathrm{d}S_t})_t$ and $(\underline{\Phi_H^t})_t$, and the resulting equation is the one of their variation forms.

Remark 3.2.11. The solution $(S_t)_t$ of (3.10) may be singular at $t = 0$, since the diagonal $\Delta = \{x, x\}_{x\in T^*Q}$ of $T^*Q \times T^*Q$ is sent by Ψ to $\{x, -x\}_{x\in T^*Q}$ which is not the graph of a globally defined differential form on $Q \times Q$. For instance, when

$$H : T^*\mathbb{R}^d \to \mathbb{R} : (q,p) \mapsto V(q) + K(p)$$

is a separable fiberwise convex Hamiltonian and f is the Legendre transform of K, $\nabla f = (\nabla K)^{-1}$ and the symplectic Euler scheme $(q,p) \mapsto (\tilde{q},\tilde{p})$ can be rewritten as:

$$\begin{cases} p = & \nabla f(\frac{q-\tilde{q}}{\epsilon}) + \epsilon\nabla V(q) & = \partial_q S_\epsilon(q,\tilde{q}) \\ \tilde{p} = & \nabla f(\frac{q-\tilde{q}}{\epsilon}) & = \partial_{\tilde{q}} S_\epsilon(q,\tilde{q}) \end{cases},$$

for $S_\epsilon(q,\tilde{q}) = \epsilon V(q) - \epsilon f(\frac{q-\tilde{q}}{\epsilon})$. Since K is convex, for any $(q,\bar{q})$ outside the diagonal,

$$\lim_{\epsilon\to 0} S_\epsilon(q,\tilde{q}) = \infty.$$

This have consequences because in numerical schemes, the step is a small number. For instance, in [23], where a formalism for fiberwise linear Poisson structures is developed, the authors get rid of the singularity by a local non-canonical change of coordinates.

Using an embedding of the local symplectic groupoid in the cotangent bundle of the unit manifold, we will see in section 3.3.2 a different kind of Hamilton-Jacobi equation for which $S_0 = 0$.

Remark 3.2.12. In theorem 3.2.10, one might replace $Q \times Q$ by a groupoid $G \rightrightarrows Q$, T^*Q by the dual A^* of the Lie algebroid of G and $T^*Q \times T^*Q$ by the cotangent groupoid $T^*G \rightrightarrows A^*$ of G. This is based on the classical observation that T^*G is a symplectic groupoid integrating the Poisson manifold A^*. Then, one would obtain theorem 7 in [23].

3.2.3 Symplectic groupoids

The Lagrangian submanifolds we are interested in lie in a neighborhood of the Poisson manifold in its symplectic groupoid, a framework that we introduce now, following [16] (see [18] for a complete review on the subject).

Definition 3.2.13. Let $\mathcal{G} \rightrightarrows M$ be a Lie groupoid over M. A symplectic 2-form $\Omega \in \Omega^2(\mathcal{G})$ is said to be multiplicative if the graph of the product

$$\Big\{(g_1, g_2, g_1.g_2) \in \mathcal{G}^3, \alpha(g_2) = \beta(g_1)\Big\}$$

is Lagrangian for the symplectic form $\mathrm{pr}_1^*\Omega + \mathrm{pr}_2^*\Omega - \mathrm{pr}_3^*\Omega$, where $\mathrm{pr}_i : \mathcal{G}^3 \to \mathcal{G}$ is the projection over the i-th factor. The pair $(\mathcal{G} \rightrightarrows M, \Omega)$ is then called a symplectic groupoid.

Let us recall some useful properties of symplectic groupoids.

1. The unit manifold M is a Lagrangian submanifold in $(\mathcal{G}, \Omega)$ and comes equipped with a natural Poisson structure π such that the source $\alpha\colon \mathcal{G} \to M$ is a Poisson map. Also the target $\beta\colon \mathcal{G} \to M$ is an anti-Poisson map.

2. The Lie algebroid of $\mathcal{G}$ is isomorphic to T^*M: its anchor is $\pi^\sharp\colon T^*M \to TM$. Its leaves are the symplectic leaves of π. Also, since a 1-form $\nu \in \Omega^1(M)$ is a section of the Lie algebroid, it defines a right-invariant vector field and a left-invariant vector field on $\mathcal{G} \rightrightarrows M$, respectively denoted by $\overrightarrow{\nu}$ and $\overleftarrow{\nu}$ and associated, under the isomorphism $\Omega^\flat\colon T\mathcal{G} \simeq T^*\mathcal{G}$, to the left and right invariant 1-forms $\alpha^*\nu$ and $\beta^*\nu$.

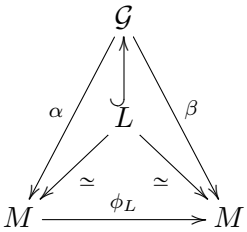
Although not every Poisson manifold (M, π) is the unit manifold of a symplectic groupoid, every Poisson manifold is the unit manifold of a local symplectic groupoid, see e.g. [19], [22], said to *integrate* (M, π). Two local symplectic groupoids integrating the same Poisson manifold are isomorphic in a neighborhood of M.

The relation between the local symplectic groupoid of a Poisson manifold and Poisson integrators comes from the following theorem about *bi-sections*, i.e. submanifolds $L \subset \mathcal{G}$ to which the restrictions of both source and target maps are diffeomorphisms onto M. Notice that any bi-section $L \subset \mathcal{G}$ induces a diffeomorphism $\phi_L := \beta_{|_L} \circ \alpha_{|_L}^{-1}$ of the unit manifold M.

Proposition 3.2.14 ([16])**.** *Let (M, π) be a Poisson manifold and $(\mathcal{G} \rightrightarrows M, \Omega)$ a local symplectic groupoid integrating it. If a bi-section $L \subset \mathcal{G}$ is Lagrangian, then:*

1. *the induced diffeomorphism $\phi_L\colon M \to M$ is a Poisson automorphism,*

2. *provided that the fibers of the source map are connected, for all $x \in M$, $\phi_L(x)$ and x belong to the same symplectic leaf.*



(3.18)

We are now interested in smooth families of Lagrangian submanifolds $(L_t)_{t\in I}$ of a symplectic groupoid $\mathcal{G}$, where $I \subset \mathbb{R}$ is an open interval containing 0, that happen to be bi-sections for all $t \in I$. From now on, such an $(L_t)_{t\in I}$ shall be refered to as a *smooth family of Lagrangian bi-sections.*

Example 3.2.15 (Lagrangian bi-sections of the symplectic groupoid of a symplectic manifold)**.** The symplectic groupoid of a symplectic manifold (M, ω) is the pair groupoid. In addition, any smooth family of symplectomorphism $(\phi_t)_t$ of a symplectic manifold (M, ω) is the flow of a time-dependent vector field related through ω to a time-dependent closed form (ξ_t). Consequently, any smooth family of Lagrangian bi-section $(L_\epsilon)_{\epsilon\in I}$ will be of the form $\{(x, \phi_\epsilon(x)), x \in M\}_{\epsilon\in I}$.

If $M = T^*Q$ is a cotangent bundle, for any solution $S \in \mathcal{C}^\infty(I \times Q \times Q)$ of Hamilton-Jacobi equation as in section 3.2.2, a smooth family of Lagrangian bi-sections of the pair groupoid $T^*Q \times T^*Q$ of T^*Q is given by $\Psi(\underline{\mathrm{d}S_t})_t$ where

$$\Psi(\underline{\mathrm{d}S_t}) = \{(\mathrm{d}_q S_t(q, \bar{q}), -\mathrm{d}_{\bar{q}} S_t(q, \bar{q})), (q, \bar{q}) \in Q \times Q\} \subset T^*Q \times T^*Q.$$

Example 3.2.16 (Lagrangian bi-sections of the symplectic groupoid of the dual of a Lie algebra)**.** Let us identify T^*G with $G \times \mathfrak{g}^*$ by left translations. This transformation groupoid integrates the canonical Poisson structure on $\mathfrak{g}^*$, where the source is the projection on $\mathfrak{g}^*$. Then any smooth family of Lagrangian bi-sections is of the form

$$\forall t,\ L_t \stackrel{\text{def}}{=} \{(\rho_t(p), p) \in T^*G, p \in \mathfrak{g}^*\}$$

where ρ is a smooth family of sections of the source such that

$$L_{(\rho_t)^{-1}*} \mathrm{d}_x \rho_t : \mathfrak{g}^* \to \mathfrak{g}$$

is symmetric for the dual pairing for all $x \in \mathfrak{g}^*$. The corresponding Poisson automorphism is $p \in \mathfrak{g}^* \mapsto \mathrm{Ad}^*_{\rho_t(p)}.p$

Remark 3.2.17. Any exact family of Lagrangian bi-sections L induces naturally a Hamiltonian Poisson integrator of timestep Δt

$$\begin{array}{rcl} M & \longrightarrow & M \\ x & \longmapsto & \beta \circ (\alpha_{|L_{\Delta t}})^{-1}(x) \end{array}$$

in the sense of the definition 3.2.25 below.

This procedure allows to construct Poisson automorphisms that not only remain in the same symplectic leaf when we iterate them but also are Hamiltonian trajectories. This is a natural property to ask to a Poisson scheme. The reader may notice that given a Hamiltonian H on M, one does not know its flow and the bi-sections $L_t = \Phi^t_{\overrightarrow{H}}(M)$ are consequently not generically computable. In section 3.3, we explain how Hamilton-Jacobi equation on the symplectic groupoid produces Lagrangian bi-sections such that the induced Poisson integrator approximates a Hamiltonian flow at any desired order in the timestep.

By Lemma 3.2.4, the variation form is a closed 1-form on L_t for all $t \in I$. Using $(\alpha^{-1}_{|_{L_t}})^* \colon \Omega^1(L_t) \to \Omega^1(M)$, the variation 1-forms of $(L_t)_{t\in I}$ become a smooth family $(\xi_t)_{t\in I}$ of closed 1-forms in $\Omega^1(M)$, that we still call *the variation* 1*-forms of* $(L_t)_{t\in I}$, with a slight abuse of notation. Before stating the proposition that relates ξ and L, denoting by $\Omega^\flat$ the musical isomorphism of the symplectic form Ω:

Lemma 3.2.18. *Let $(L_t)_{t\in I}$ and $(\xi_t)_{t\in I}$ be as above. The time t-flow of the time dependent vector field $\overrightarrow{\xi_t} = (\Omega^\flat)^{-1}(\alpha^*\xi_t)$ restricts to a diffeomorphism from L_0 to L_t.*

Proof. By definition of variation forms, $\Phi^t_{\overrightarrow{\xi}}(L_0) \subset L_t$. In order to prove the other inclusion, let $x \in L_t$ and set $x_0 = (\Phi^t_{\overrightarrow{\xi}})^{-1}(x)$. We are left to prove that $x_0 \in L_0$. Since the flow of $\overrightarrow{\xi}$ is an L-path, $\overrightarrow{\xi}$ is a complete vector field on I and (3.9) ensures that the flow $\Phi_{\overrightarrow{\xi}}$ is locally an L-path:

$$\forall\ 0 \leqslant u \leqslant t, \exists\ \epsilon_0 > 0, \forall\ |\epsilon| \leqslant \epsilon_0, \Phi^{u-\epsilon}_{\overrightarrow{\xi}}(x_0) \in L_{u-\epsilon}$$

For any $u \in [0, t]$, $(\Phi^u_{\overrightarrow{\xi}})^{-1}(x) \in L_u$, hence the result. □

Lemma 3.2.18 says that smooth families $(L_t)_{t\in I}$ of Lagrangian bi-sections in a symplectic groupoid can be recovered from L_0 and from their associated variation forms $(\xi_t) \in Z^1(M)$. Not every pair $(L_0, (\xi_t))$ gives a family of Lagrangian bi-sections, because the flow of $\overrightarrow{\xi_t}$ may not be defined for every time $t \in I$. However, the correspondence works under relatively mild assumptions:

Proposition 3.2.19. *Let I be an interval containing 0. In a symplectic groupoid $\mathcal{G} \rightrightarrows M$, there is a one-to-one correspondence between:*

(i) smooth families of Lagrangian bi-sections $(L_t)_{t\in I}$ of $(\mathcal{G}, \Omega)$,

(ii) pairs made of a Lagrangian bi-section L_0 and a smooth family of closed one-forms on the base $(\xi_t)_{t\in I}$ such that the vector field $\pi^\#(\xi_t)$ is a complete vector field on M.

Proof of Proposition 3.2.19. From lemma 3.2.18, for any $\epsilon \in I$,

$$L_\epsilon = \phi^\epsilon_{\overrightarrow{(\xi_t)_t}}(L_0). \tag{3.19}$$

Consequently, two smooth families of Lagrangian bi-sections admitting the same variation forms and corresponding at 0 are equal.

Now, set $L_\epsilon = \phi^\epsilon_{\overrightarrow{(\xi_t)_t}}(L_0)$. The smoothness and bi-section properties are clear. We prove that L_ϵ is a Lagrangian submanifold.
Indeed, the flow of a left-invariant vector field is a symplectomorphism if and only if the corresponding 1-form on the base is closed. To verify this claim, set $\Pi \in \Gamma(\Lambda^2\mathcal{G})$ the Poisson tensor corresponding to Ω. For any $f, g \in \mathcal{C}^\infty(M)$, using the Schouten bracket of [22]:

$$\begin{aligned}\mathscr{L}_{\overrightarrow{f.\mathrm{d}g}}\Pi &= \alpha^* f \mathscr{L}_{\overrightarrow{\mathrm{d}g}}\Pi + \overrightarrow{\mathrm{d}f} \wedge \overrightarrow{\mathrm{d}g} \\ &= \overrightarrow{\mathrm{d}f \wedge \mathrm{d}g} \\ &= \overrightarrow{\mathrm{d}(f\mathrm{d}g)}.\end{aligned}$$

Then:

$$\mathscr{L}_{\overrightarrow{\xi_\epsilon}}\Pi = \overrightarrow{\mathrm{d}\xi_\epsilon} = 0 \tag{3.20}$$

concludes the proof. □

Remark 3.2.20. Equation (3.19) proves that a smooth family of Lagrangian bi-sections $(L_t)_{t\in I}$ is exact if and only if there exist global L-paths that are left-invariant time-dependent Hamiltonian trajectories:

$$\exists\, H \in \mathcal{C}^\infty(M \times \mathbb{R}), \forall\, t_0 \in I, \forall\, x \in L_{t_0}, \exists\, \gamma \text{ an L-path, } \begin{cases} \gamma(t_0) = x \\ \dot\gamma = X_{\alpha^* H}(\gamma) \end{cases}$$

Remark 3.2.21. Equation (3.20) comes out from the multiplicativity of Π and is a particular case of a much more general correspondence between multiplicative polyvector fields on the groupoid and differentials on its algebroid, cf. theorem 2.34 of [74].

Examples will be given in Section 3.2.5, except for the following two examples, that connect with symplectic geometry.

Example 3.2.22. The example 3.2.15 already relates smooth family of closed 1-forms on a symplectic manifold with smooth family of Lagrangian bi-sections of the associated pair groupoid.

Example 3.2.23. According to Weinstein's theorem [16], every Poisson manifold (M, π) integrates to a local symplectic groupoid structure $(\mathcal{G} \rightrightarrows M, \omega)$ where $\mathcal{G}$ is a neighborhood $\mathfrak{U}(M)$ of the zero section of T^*M and $\omega = \omega_{can}$ is the restriction to $\mathfrak{U}(M)$ of the canonical symplectic 2-form of T^*M. To every smooth family (L_t) of Lagrangian bi-sections with $L_0 = M$ and $L_t \subset \mathfrak{U}(M)$, we can therefore associate two different kinds of families of closed 1-forms.

1. We can forget the groupoid structure, and say that on T^*M, each one of the L_t is the graph of a closed 1-form:
$$L_t = \{\zeta_t|_m, m \in M\}$$
for ζ_t a closed 1-form on M.

2. Alternatively, one can forget that $\mathcal{G}$ has been identified to T^*M, and use Proposition 3.2.19 to associate a family ξ_t of closed 1-forms.

Both families of closed 1-forms are in general different, but related by the equality of the variation forms of their corresponding families of Lagrangian submanifolds. As 1-forms on L_t for all t:
$$\alpha^*\xi_t = \tau^*\frac{d\zeta_t}{dt}$$
where $\tau\colon T^*M \to M$ is the natural projection.

3.2.4 Hamiltonian Poisson integrators and their backward analysis

Poisson integrators appearing in the literature may be understood as germs of Lagrangian bi-sections. A particular case of this principle is developed for fiberwise linear Poisson structures on the dual of a Lie algebroid in [23].

Let us consider a Hamiltonian vector field, i.e. a differential equation of the type
$$\dot{x}(t) = \pi^{\#}_{x(t)}(d_{x(t)}H) = X_H|_{x(t)}$$
where (M, π) is a Poisson manifold and $H \in \mathcal{C}^\infty(M)$ a Hamiltonian function. A reasonable definition of a *Poisson integrator* ϕ_ϵ *of order* $k \geqslant 1$ *for* H might be defined by the following three conditions :

1. ϕ_ϵ agrees with the time-ϵ flow of X_H up to order k in ϵ,

2. ϕ_ϵ is a Poisson diffeomorphism for all $\epsilon \in I$,

3. ϕ_ϵ maps each leaf to itself (through a map which is necessarily a symplectic diffeomorphism).

The purpose of a Poisson integrator is to choose a particular value Δt of ϵ, called *timestep*, then consider the iterations of the diffeomorphism $\phi_{\Delta t}$. The hope is of course that the n-th iterations remain good approximations of the flow of X_H at time $n\Delta t$ for large $n \in \mathbb{N}$.

In the particular case of symplectic integrators, the theoretical ground of their good behaviour is their backward analysis. Indeed, any smooth family of symplectomorphisms $(\phi_t)_t$ is the flow of a time-dependent vector field $(X_t)_t$ related through the symplectic form to the flow of a closed 1-form. So any symplectic integrator for H at order k is locally the flow of a time-dependent Hamiltonian $(h_t)_t$ such that $h_0 = H$. The order k of the method is then related to the order at which the initial Hamiltonian H equals $(h_t)_t$: $H = h_t + o\big(t^{k-1}\big)$.

In this context, an important feature of Poisson integrators is that it is not always true anymore. There exists a smooth family of Poisson automorphisms, even staying on the same symplectic leaf, that are not a flow of a time-dependent Hamiltonian, because of so-called outer-automorphisms. These are measured by the first Poisson cohomology group of the Poisson manifold. This makes a huge difference with symplectic schemes, for which this property is automatically verified, at least locally. Here is an example of such a phenomenon:

Example 3.2.24. For the Poisson tensor $\pi = (x^2 + y^2)\partial_x \wedge \partial_y$ on $\mathbb{R}^2$, a Poisson integrator for $H : (x, y) \to \frac{x^2+y^2}{2}$ of order k and step Δt is

$$\begin{pmatrix} x_{n+1} \\ y_{n+1} \end{pmatrix} = e^{(\Delta t)^k} \begin{pmatrix} \cos r_n \Delta t & -\sin r_n \Delta t \\ \sin r_n \Delta t & \cos r_n \Delta t \end{pmatrix} \cdot \begin{pmatrix} x_n \\ y_n \end{pmatrix} \text{ where } r_n = (x_n)^2 + (y_n)^2 \tag{3.21}$$

and behaves remarkably bad for long simulations: for any norm $\|.\|$ and initial point $(x_0, y_0) \neq 0_{\mathbb{R}^2}$, denoting by Φ_H the flow of the Hamiltonian vector field generated by H,

$$\|(x_n, y_n) - \Phi_H^{n\Delta t}(x_0, y_0)\| \underset{n\to+\infty}{\longrightarrow} +\infty.$$

As in the general case, this phenomenon is explained by the fact that the first Poisson cohomology group H^1_π is locally non-trivial around 0: there exists no neighborhood U of 0 such that $H^1_\pi(U) = \{0\}$. Indeed, H^1_π is generated by rotations and dilations. In other words, there exist smooth families of Poisson automorphisms $(\phi_t)_t$ such that $\phi_0 = \mathrm{Id}$ but ϕ is not the flow of a time-dependent Hamiltonian vector field.

The previous example suggests to make stronger assumptions to define a notion of Hamiltonian Poisson integrator:

Definition 3.2.25 (Hamiltonian Poisson integrator)**.** Let (M, π) a Poisson manifold and $H \in \mathcal{C}^\infty(M)$ a Hamiltonian on M. A smooth family $(\phi_\epsilon)_{\epsilon\in I}$ of diffeomorphisms of M is a *Hamiltonian Poisson integrator of order $k \geqslant 1$ for H* if:

1. ϕ_ϵ is a Poisson diffeomorphism for all $\epsilon \in I$,
2. there exists $(h_t)_t$ a time-dependent Hamiltonian such that
   (a) $h_t = H + o\big(t^{k-1}\big)$
   (b) $\phi_\epsilon = \Phi^\epsilon_{(h_t)_t}$ is the time-ϵ flow of h.

It follows easily that

$$\phi_\epsilon = \Phi^\epsilon_H + o\Big(\epsilon^k\Big) \tag{3.22}$$

in the sense of theorem 3.1.5 and related Magnus series.

We can now state the main result of this section, which is the core of the explicit constructions of Poisson integrators that will be presented in the sequel. We recall that given an exact family of Lagrangian bi-sections L on $(\mathcal{G} \rightrightarrows M, \omega)$, their variation functions $(h_t)_t \in \mathcal{C}^\infty(M \times I)$ denote the pull-back by the source of exact 1-forms obtained from L-paths through ω.

Theorem 3.2.26. *Let (M, π) be a Poisson manifold, $(\mathcal{G} \rightrightarrows M, \omega)$ a local symplectic groupoid integrating it and $k \geqslant 1$. For every smooth family $(L_t)_{t\in I}$ of exact Lagrangian bi-sections such that $L_0 = M$ and with variation functions $(h_t)_{t\in I}$, if the Magnus series $\mathcal{M}_\epsilon(h)$ of $(h_t)_{t\in I} \in \mathcal{C}^\infty(M \times I)$ coincides with ϵH at order k, then the induced family of diffeomorphisms $(\phi_{L_t})_{t\in I}$ is a Hamiltonian Poisson integrator of order k for H.*

Remark 3.2.27. We invite the reader to understand Theorem 3.2.26 as meaning that, provided a symplectic groupoid integrating a Poisson structure is entirely known and computable, then finding a Hamiltonian Poisson integrator reduces to a Magnus series question. This is the first part of the construction we have announced in the introduction.

Proof of theorem 3.2.26. Since ϕ is induced by L, it is a Hamiltonian Poisson integrator for H, of time-dependent Hamiltonian $(h_t)_{t\in I}$.
We still need to compute its order. For any $f \in \mathcal{C}^\infty(M)$:

$$\begin{aligned}\phi_\epsilon^* f &= (\Phi^\epsilon_{(h_t)_{t\in I}})^* f \\ &= (\Phi^1_{\epsilon H})^* f + o\Big(\epsilon^k\Big) \\ &= (\Phi^\epsilon_H)^* f + o\Big(\epsilon^k\Big)\,.\end{aligned}$$

This concludes the proof. □

Corollary 3.2.28. *Let (M,π) be a Poisson manifold and $(\mathcal{G} \rightrightarrows M, \omega)$ a local symplectic groupoid integrating it.*

For every smooth family $(L_t)_{t\in I}$ of exact Lagrangian bi-sections with $L_0 = M$, if the corresponding variation form at 0 $\frac{\partial L_t}{\partial t}\big|_{t=0}$ is equal to dH, then its induced diffeomorphisms $(\phi_{L_t})_{t\in I}$ are Hamiltonian Poisson integrators of order 1 for H.

3.2.5 Examples of Hamiltonian Poisson integrators

The description of Poisson integrators in Theorem 3.2.26 unifies already known constructions: the classical Euler-Symplectic scheme [32] (see Example 3.2.29), the mid-point method for the harmonic oscillator (see Example 3.2.30), and the Kahan discretization of Lotka-Volterra system already described by Pol Vanhaecke [41] (see Example 3.2.32).

Example 3.2.29 (Euler symplectic scheme for a separable Hamiltonian)**.** For a general Hamiltonian $H \in \mathcal{C}^\infty(T^*\mathbb{R}^d)$ and (q,p) cotangent coordinates, the symplectic Euler scheme ([32]) is:

$$\begin{cases} q_{n+1} = q_n + \Delta t \frac{\partial H}{\partial p}(q_n, p_{n+1}) \\ p_{n+1} = p_n - \Delta t \frac{\partial H}{\partial q}(q_n, p_{n+1}) \end{cases}. \tag{3.23}$$

Let us interpret this implicit (in the generic case) numerical scheme as a Poisson integrator at order 1 for H, in the sense of theorem 3.2.26. We use the notations of the latter theorem:

(M,ω) On $M = T^*\mathbb{R}^d$, we denote by (q,p) some canonical cotangent coordinates, and we consider the canonical Poisson structure associated to the symplectic 2-form $\omega = \sum_{i=1}^d dp_i \wedge dq_i$.

$(\mathcal{G},\Omega)$ the symplectic groupoid integrating the Poisson manifold $T^*\mathbb{R}^d$ is the pair groupoid $\mathcal{G} := T^*\mathbb{R}^d \times T^*\mathbb{R}^d$ equipped with the subtraction of canonical symplectic forms $\Omega = \sum_{i=1}^d dp_i \wedge dq_i - \sum_{i=1}^d d\tilde{p}_i \wedge d\tilde{q}_i$, $(\tilde{q},\tilde{p})$ some canonical cotangent coordinates on the second factor.

(L_ϵ) The submanifold

$$L_\epsilon = \left\{(q,p,\tilde{q},\tilde{p}),\ \tilde{q} = q + \epsilon\frac{\partial H}{\partial p}(q,\tilde{p}) \text{ and } \tilde{p} = p - \epsilon\frac{\partial H}{\partial q}(q,\tilde{p})\right\}$$

is Lagrangian in $(\mathcal{G},\Omega)$. Indeed, using relations on L_ϵ:

$$\mathrm{d}\tilde{p} \wedge \mathrm{d}\tilde{q} = \mathrm{d}p \wedge \mathrm{d}q + \epsilon \mathrm{d}p \wedge \mathrm{d}\frac{\partial H}{\partial p}(q,\tilde{p}) - \epsilon \mathrm{d}\frac{\partial H}{\partial q}(q,\tilde{p}) \wedge \mathrm{d}q - \epsilon^2 \mathrm{d}\frac{\partial H}{\partial q}(q,\tilde{p}) \wedge \mathrm{d}\frac{\partial H}{\partial p}(q,\tilde{p}). \tag{3.24}$$

The term $\mathrm{d}\frac{\partial H}{\partial q}(q,\tilde{p}) \wedge \mathrm{d}\frac{\partial H}{\partial p}(q,\tilde{p})$ vanishes because the graph of $\mathrm{d}H$ is Lagrangian and $\mathrm{d}p \wedge \mathrm{d}\frac{\partial H}{\partial p}(q,\tilde{p}) = \mathrm{d}\frac{\partial H}{\partial q}(q,\tilde{p}) \wedge \mathrm{d}q$ by symmetry of the Hessian matrix, so that $\mathrm{d}\tilde{p} \wedge \mathrm{d}\tilde{q} = \mathrm{d}p \wedge \mathrm{d}q$.

For ϵ small enough, it is also a bi-section of $\mathcal{G}$, at least after restriction to a relatively compact open subset. To simplify the presentation, we will assume that it is a globally defined bi-section. For $\epsilon = 0$, the bi-section is the unit manifold $M = T^*\mathbb{R}^d$.

(ϕ_ϵ) The bi-sections L_ϵ define a smooth family of symplectomorphisms of $(M = T^*\mathbb{R}^d, \omega)$, which are precisely, for $\epsilon = \Delta t$, the symplectic Euler Poisson integrator (3.23).

$(h_t, \mathbf{H}_\epsilon)$ Under the simplifying assumption that H is separable, i.e. it splits in the following form:

$$H : T^*\mathbb{R}^d \to \mathbb{R} : (q,p) \mapsto V(q) + K(p)$$

with V and K two smooth real-valued functions, we can compute explicitely:

the variation functions i.e.

$$h_t \colon (q,p) \mapsto K(p) + V\left(q + t\frac{\partial K}{\partial p}(p)\right) \tag{3.25}$$

and the modified Hamiltonian, i. e. the Magnus series of h_t, has first two terms

$$\mathbf{H}_\epsilon := \epsilon H + \frac{\epsilon^2}{2}\left\langle \frac{\partial V}{\partial q}, \frac{\partial K}{\partial p} \right\rangle + o(\epsilon^2) \tag{3.26}$$

Let us explain how we computed (3.25). Under the assumption that H splits, the Lagrangian submanifold corresponding to (3.23) becomes

$$\begin{cases} \tilde{q} = q + \epsilon\frac{\partial K}{\partial p}(p - \epsilon\frac{\partial V}{\partial q}) \\ \tilde{p} = p - \epsilon\frac{\partial V}{\partial q}(q) \end{cases} . \tag{3.27}$$

Using the relations

$$\begin{cases} q = \tilde{q} - \epsilon\frac{\partial K}{\partial p}(\tilde{p}) \\ p = \tilde{p} + \epsilon\frac{\partial V}{\partial q}(\tilde{q} - \epsilon\frac{\partial K}{\partial p}(\tilde{p})) \end{cases} , \tag{3.28}$$

the differentiation of the L-path $\phi_\epsilon = \begin{pmatrix} \tilde{q} \\ \tilde{p} \end{pmatrix}$ with respect to ϵ gives :

$$\partial_\epsilon \begin{pmatrix} \tilde{q} \\ \tilde{p} \end{pmatrix} = \begin{pmatrix} \frac{\partial K}{\partial p}(\tilde{p}) - \epsilon\frac{\partial^2 K}{\partial p^2}(\tilde{p}) \cdot \frac{\partial V}{\partial q}(\tilde{q} - \epsilon\frac{\partial K}{\partial p}(\tilde{p})) \\ \frac{\partial V}{\partial q}(\tilde{q} - \epsilon\frac{\partial K}{\partial p}(\tilde{p})) \end{pmatrix} = \begin{pmatrix} \partial_p h_\epsilon(\tilde{q},\tilde{p}) \\ -\partial_q h_\epsilon(\tilde{q},\tilde{p}) \end{pmatrix}$$

and the system (3.23) is consequently Hamiltonian with respect to the time-dependent Hamiltonian $(h_t)_{t\in I}$.

Example 3.2.30 (Mid-point scheme)**.** For this example, the Hamiltonian is the harmonic oscillator $H \colon (q,p) \mapsto \frac{1}{2}(\|q\|^2 + \|p\|^2)$, for which it is well-known ([32]) that the mid-point scheme

$$\begin{cases} q_{n+1} = q_n + \Delta t\frac{p_n + p_{n+1}}{2} \\ p_{n+1} = p_n - \Delta t\frac{q_n + q_{n+1}}{2} \end{cases} ,$$

is symplectic.

(M, ω) The Poisson manifold $M = T^*\mathbb{R}^d$ is the same as the last example.

$(\mathcal{G}, \Omega)$ As a consequence, the symplectic groupoid $T^*\mathbb{R}^d \times T^*\mathbb{R}^d$ does not differ as well.

(L_ϵ) For any $\epsilon \in \mathbb{R}$, the submanifold

$$L_\epsilon = \left\{ (q,p,\tilde{q},\tilde{p}),\ \tilde{q} = q + \epsilon\frac{p+\tilde{p}}{2} \text{ and } \tilde{p} = p - \epsilon\frac{q+\tilde{q}}{2} \right\}$$

is a Lagrangian bi-section in $(\mathcal{G}, \Omega)$. That can be seen using relations on L_ϵ :

$$\begin{cases} \tilde{q} &= \frac{1}{1+\frac{\epsilon^2}{4}}(\epsilon p + (1-\frac{\epsilon^2}{4})q) \\ \tilde{p} &= \frac{1}{1+\frac{\epsilon^2}{4}}(-\epsilon q + (1-\frac{\epsilon^2}{4})p) \end{cases} \tag{3.29}$$

and consequently

$$\mathrm{d}\tilde{p} \wedge \mathrm{d}\tilde{q} = \frac{1}{(1+\frac{\epsilon^2}{4})^2}(-\epsilon^2 \mathrm{d}q \wedge \mathrm{d}p + (1-\frac{\epsilon^2}{4})^2 \mathrm{d}p \wedge \mathrm{d}q) \tag{3.30}$$

$$= \mathrm{d}p \wedge \mathrm{d}q. \tag{3.31}$$

($h_t, \mathbf{H}_\epsilon$) The above one-step forward map $\phi_t \colon (q,p) \mapsto (\tilde{q},\tilde{p})$ induces a vector field $X_t = \partial_t \phi_t \circ \phi_t^{-1}$. One verifies that X_t is colinear to the Hamiltonian vector field of H, and so are H and the time-dependent Hamiltonian: expressing $\frac{\mathrm{d}\tilde{q}}{\mathrm{d}\epsilon}$ and $\frac{\mathrm{d}\tilde{p}}{\mathrm{d}\epsilon}$ with respect to $\tilde{q}$ and $\tilde{p}$, on computes the Hamiltonian vector field of $(h_t)_t$ and consequently $(h_t)_t$: at a time t,

$$h_t(q,p) = \frac{(1-\frac{t^2}{4})^2 + t^2}{(1+\frac{t^2}{4})^3} H(q,p).$$

The modified Hamiltonian is simply

$$\mathbf{H}_\epsilon = \int_0^\epsilon \frac{(1-\frac{t^2}{4})^2 + t^2}{(1+\frac{t^2}{4})^3} \mathrm{d}t \times H.$$

In this case, the Hamiltonian Poisson integrator preserves H.

Example 3.2.31 (Linear Hamiltonian on the dual of a Lie algebra)**.** Let G be a Lie group, $\mathfrak{g}$ its Lie algebra and consider its symplectic groupoid $G \times \mathfrak{g}^* \rightrightarrows \mathfrak{g}^*$. As the coadjoint action of G on $\mathfrak{g}^*$ preserves the Lie bracket, a Poisson scheme discretising the flow of a linear Hamiltonian $f \in \mathfrak{g}$ is given by:

$$x_{n+1} = \mathrm{Ad}^*_{\exp(\epsilon f)} x_n$$

and corresponds to the Lagrangian bi-sections $\{(\exp(\epsilon f), x), x \in \mathfrak{g}^*\} \subset G \times \mathfrak{g}^*$.

Example 3.2.32 (Kahan discretization of one Lotka-Volterra system)**.** For the quadratic Poisson bracket on $\mathbb{R}^d$ given by:

$$\{x_i, x_j\} = x_i x_j \text{ if } 1 \leqslant i < j \leqslant d \tag{3.32}$$

and the linear Hamiltonian $H(x) = \sum_{i=1}^d x_i$, a Poisson integrator is given in [41] by the Kahan discretisation

$$x_i^{(n+1)} - x_i^{(n)} = \Delta t\, x_i^{(n)} \Big(\sum_{j>i} x_j^{(n+1)} - \sum_{j<i} x_j^{(n+1)} \Big) + \Delta t\, x_i^{(n+1)} \Big(\sum_{j>i} x_j^{(n)} - \sum_{j<i} x_j^{(n)} \Big) \tag{3.33}$$

where n is the iteration indice of the scheme and $x = (x_i)$ are coordinates on $\mathbb{R}^d$.

Let us interpret this discretization in terms of Theorem 3.2.26 and show that it is a Hamiltonian Poisson intergator:

(M,π) is $M=\mathbb{R}^d$ with the Poisson structure (3.32).

$(\mathcal{G},\Omega)$ Its symplectic groupoid is

$\mathcal{G}=T^*\mathbb{R}^d$,
$\Omega=\sum_i \mathrm{d}x_i\wedge\mathrm{d}p_i+\sum_{i,j}(\delta_{i<j}-\delta_{i>j})x_ip_j\mathrm{d}x_i\wedge\mathrm{d}p_j+\sum_{j<i}p_ip_j\mathrm{d}x_i\wedge\mathrm{d}x_j+\sum_{j<i}x_ix_j\mathrm{d}p_i\wedge\mathrm{d}p_j$
$\alpha\colon(x,p)\mapsto x$,
$\beta\colon(x,p)\mapsto\left(e^{\sum_i(\delta_{i<j}-\delta_{i>j})x_ip_i}x_j\right)_{1\leqslant j\leqslant n}$

with (x,p) cotangent coordinates on $T^*\mathbb{R}^d$.

(h_t) The variation function is given by:

$$h_t(x)=H(x)\times\frac{\partial f}{\partial t}(t,H(x)),$$

where[2]

$$\begin{array}{rccc} f & : & (\mathbb{R},0)\times\mathbb{R} & \to & \mathbb{R} \\ & & (t,u) & \mapsto & \frac{2}{u}\mathrm{arctanh}(tu) \end{array}.$$

(L_ϵ) The family of Lagrangian submanifolds L_ϵ are given by $L_\epsilon=\Phi^\epsilon_{(\alpha^*h_t)_{t\in\mathbb{R}}}(\mathbb{R}^d)$.

L_0 is the unit manifold.

(ϕ_ϵ) The induced Poisson diffeomorphism is defined implicitly by (3.33) for $\epsilon=\Delta t$.

(H_ϵ) The modified Hamiltonian is simply $\mathbf{H}_\epsilon(x):=H(x)f(\epsilon,H(x))$.

Let us give some details on these points.

Let ϕ_ϵ the map implicitly defined by equation (3.33) and $f\colon\begin{array}{ccc}(\mathbb{R},0)\times\mathbb{R} & \to & \mathbb{R}\\ (t,u) & \mapsto & \frac{e^{ut}-1}{u(e^{ut}+1)}\end{array}$. Then following proposition 3.1 of [41],

$$\phi_\epsilon(x)=\Phi_H^{f(t,x)}(x). \tag{3.34}$$

In this case, one verifies by differentiation that

$$\Phi_h^t(x)=\Phi_H^{f(t,H(x))}(x) \tag{3.35}$$

where

$$h_t(x)=H(x)\times\frac{\partial f}{\partial t}(t,H(x)).$$

The Lagrangian bi-sections associated to (3.33) are the image of $\mathbb{R}^d$ by the flows of the time-dependent right-invariant vector fields associated to $(\mathrm{d}h_t)_{t\in I}$ in the symplectic groupoid integrating $(\mathbb{R}^d,\{.,.\})$.

Example 3.2.33 (Splitting methods through Lagrangian bi-sections)**.** This example is inspired by [39]. Let $\mathcal{G}\rightrightarrows M$ be a symplectic groupoid integrating a Poisson manifold M and $H=H_1+H_2$ be a splitted Hamiltonian such that for each H_i, one knows a smooth family of Lagrangian bi-sections $(L^i_t)_t$ inducing a Poisson integrator $(\phi^i_\epsilon)_\epsilon$ for H_i at order 1, with variation functions $(h^i_t)_t$.

[2] All along this manuscript, the notation $(\mathcal{T},x)$ stands for a neighborhood of x in its topological space $\mathcal{T}$.

(L_ϵ) The composition of Lagrangian bi-sections in $\mathcal{G}$, as detailed in appendice .1, is a Lagrangian bi-section again, so that

$$t \mapsto L^2_t \circ L^1_t$$

is a smooth family of Lagrangian bi-sections. It is easily checked to induce a Poisson integrator for H at order 1.

(ϕ_ϵ) The induced Poisson diffeomorphism is the composition $\phi_\epsilon = \phi^1_\epsilon \phi^2_\epsilon$.

(h_t) The variation function is given by

$$h_t = h^1_t + h^2_t\big((\phi^1_t)^{-1}\big)$$

and is equal to H at order 1.

For Poisson integrator at order k, the situation is more complicated. As shown by [39] in the symplectic context, we then have to compose several times the bi-sections, and use the following consequence of the Baker-Campbell-Hausdorff formula: assume we are given ϕ^1 and ϕ^2 two Poisson integrators for H_1 and H_2 at order 1, then there exists $n \in \mathbb{N}$ and $(c^j_l)_{\substack{j=1,2 \\ 1 \leqslant l \leqslant n}}$ such that $L^{(k)}_\epsilon = \Pi^1_{l=n} L^2_{c^2_l \epsilon} \circ L^1_{c^1_l \epsilon}$ induces a Poisson integrator for H at order k.

(L_ϵ) Lagrangian bi-sections are $L^{(k)}_\epsilon = \Pi^1_{l=n} L^2_{c^2_l \epsilon} \circ L^1_{c^1_l \epsilon}$.

(ϕ_ϵ) The induced Poisson diffeomorphism is the composition $\phi_\epsilon = \Pi^n_{l=1} \phi^1_{c^1_l \epsilon} \phi^2_{c^2_l \epsilon}$.

(h_t),(H_ϵ) The variation function is

$$h_t = c^1_1 h^1_t + c^2_1 h^2_t (\phi^1_{c^1_1 t})^{-1} + c^1_2 h^1_t (\phi^1_{c^1_1 t} \phi^2_{c^2_1 t})^{-1} + \dots$$

and equals H at order $k-1$. The modified Hamiltonian is the Magnus series $\mathcal{M}(h)$ of $(h_t)_t$.

3.3 Hamilton-Jacobi equation on the local symplectic groupoid

When the local symplectic groupoid is known, i.e. a symplectomorphism with a neighborhood of the zero section of T^*M (equipped with its canonical symplectic structure) is explicitly given, constructive Poisson integrator of arbitrary order for an arbitrary Hamiltonian can be given. This will turn results of section 3.2 into more constructive ones. Indeed, we have constructed in the previous examples the exact family of Lagrangian bi-sections by hand. We will now give a general manner to do it.

3.3.1 Geometry of Lagrangian bi-sections in the cotangent bundle of the base

Let us recall a classical result of Poisson geometry:

Theorem 3.3.1. *[16]-[19]-[22] There exists a neighborhood of T^*M that carries a structure of local symplectic groupoid $\mathcal{G}$ on the base M. Its symplectic form is the canonical one and its unit map is the zero section.*

Remark 3.3.2. In the above references, the symplectic form on a neighborhood of T^*M is not the canonical one. However, the base being Lagrangian, Moser's trick applies near the zero section and gives a symplectomorphism that maps the obtained symplectic forms to the canonical symplectic form. Besides, provided some local coordinates on M are fixed, [37] contains formulae constructing source and target for ω_{can} that have been recently revisited in [9] in the context of quantization. A geometric interpretation of forms obtained by Poisson sprays allows to construct wide classes of new examples of the present theory ([15]).

This theorem is, in its general form, an existence theorem. However, in many cases, the source and target maps of the groupoid structure on (T^*M, ω_{can}) can be made explicit.

Definition 3.3.3. We call a *bi-realisation* of a Poisson manifold (M, π) a triple $(\mathcal{W}, \alpha, \beta)$ made of a neighborhood $\mathcal{W} \subset T^*M$ of the zero section of T^*M symplectomorphic to a local symplectic groupoid integrating (M, π) such that the identity section of the local groupoid and the zero section of T^*M correspond by this symplectomorphism and whose source and target are α and β.

Remark 3.3.4. Notice that, as explained in section 3.2.3, for any bi-realisation $(\mathcal{W}, \alpha, \beta)$, the source $\alpha\colon \mathcal{W} \to M$ is a Poisson submersion and the target $\beta\colon \mathcal{W} \to M$ an anti-Poisson submersion. Also, it follows from the definition that α and β are left inverses of the zero section $0\colon M \to T^*M$:

$$0^*\alpha = 0^*\beta = \mathrm{Id}_M. \tag{3.36}$$

The reader may observe too that we do not specify the groupoid product.

Let us illustrate the notion of bi-realisation in some cases of interest. We make use of the so-called *Poisson spray* of [19] and Moser's trick in a neighborhood of M to compute bi-realisations of examples 3.3.5 and 3.3.8.

Example 3.3.5. For the Poisson structure $\partial_p \wedge \partial_q$ of $T^*\mathbb{R}^n$ with coordinates (q, p), denoting (q, p, ξ_q, ξ_p) the induced coordinates on $T^*T^*\mathbb{R}^n$, the choice of the Poisson spray $\xi_p\partial_q - \xi_q\partial_p$ gives the following bi-realisation:

$$\begin{cases} \alpha : (q, p, \xi_q, \xi_p) \mapsto (q - \frac{1}{2}\xi_p, p + \frac{1}{2}\xi_q) \\ \beta : (q, p, \xi_q, \xi_p) \mapsto (q + \frac{1}{2}\xi_p, p - \frac{1}{2}\xi_q) \end{cases} \tag{3.37}$$

Example 3.3.6. When (M, ω_M) is symplectic, there is no "natural" (i.e. preferred) way to send symplectically a neighborhood of the diagonal of the pair groupoid $(M \times M, p_1^*\omega_M - p_2^*\omega_M)$ on a neighborhood of M in T^*M. More precisely, there are as many ways as choices of Lagrangian bundles such that fibers are transverse to the diagonal in $M \times M$. In fact, bi-realisations are in one-to-one correspondence with symplectomorphisms between a neighborhood of the zero section in T^*M and a neighborhood of the diagonal in $M \times M$. However, they may not be computable explicitly in general.

Example 3.3.7. Let G be a Lie group with Lie algebra $\mathfrak{g}$. Consider φ a diffeomorphism from an open subset $U \subset G$ to an open subset of $\mathfrak{U} \subset \mathfrak{g}$ mapping 1_G to 0 and such that its differential at 1_G is the identity.

Since φ is a diffeomorphism, $T\varphi\colon TU \to T\mathfrak{U}$ is an invertible vector bundle morphism, and so is its cotangent lift $T^*\varphi\colon T^*\mathfrak{U} \to T^*U$. It is moreover a symplectomorphism, when $T^*\mathfrak{U}$ and T^*U are equipped with their respective canonical structures. Since the source and target of $T^*G \simeq \mathfrak{g}^* \times G$ are given by $\alpha\colon (\xi, g) \mapsto \xi$ and $\beta\colon (\xi, g) \mapsto Ad_g^*\xi$, it suffices to transport those through $T^*\varphi$ to get a bi-realisation.

Let us be more explicit: with the cotangent lift

$$T^*\varphi : \underset{\xi_x}{T^*\mathfrak{g}} \underset{\mapsto}{\to} \underset{{}^t(d_{\varphi^{-1}x}\varphi).\xi_x}{T^*G}$$

and the natural[3] isomorphism $T^*\mathfrak{g} \simeq T^*\mathfrak{g}^*$, the symplectic groupoid of the dual of a Lie algebra $T^*G \rightrightarrows \mathfrak{g}^*$ becomes indeed $\mathfrak{g} \times \mathfrak{g}^*$ near $\mathfrak{g}^*$ with source and target:

$$\begin{cases} \alpha : (\mathfrak{g}, 0) \times \mathfrak{g}^* \to \mathfrak{g}^* : (\eta, \xi) \mapsto \left({L_{\varphi^{-1}(\eta)}}^* T^*_{\varphi^{-1}(\eta)}\varphi \right).\xi \\ \beta : (\mathfrak{g}, 0) \times \mathfrak{g}^* \to \mathfrak{g}^* : (\eta, \xi) \mapsto \left({R_{\varphi^{-1}(\eta)}}^* T^*_{\varphi^{-1}(\eta)}\varphi \right).\xi \end{cases} \tag{3.38}$$

The most natural diffeomorphism φ is of course the logarithm map $\log : G \to \mathfrak{g}$. There are however other ones, like, e.g.:

1. for $\mathfrak{g}$ the Lie subalgebra of $n \times n$ nilpotent matrices, the map $\varphi\colon x \to x - \mathrm{id}$
2. for $\mathfrak{g}$ the Lie subalgebra of skew-symmetric $n \times n$ matrices, the map $x \mapsto 4\frac{\mathrm{id}-x}{\mathrm{id}+x}$ is also a diffeomorphism in a neighborhood of id.

Those are better from a computational point of view.

Example 3.3.8. The symplectic groupoid $\mathcal{G} \rightrightarrows \mathbb{R}^n$ of the real log-canonical Poisson bracket on $\mathbb{R}^n$, i.e.:

$$\{x_i, x_j\} = a_{ij} x_i x_j, \tag{3.39}$$

with $A = (a_{ij})_{i,j}$ a skew-symmetric matrix is computed in [46] and is shown to be globally diffeomorphic to $T^*\mathbb{R}^n$. The explicit structures given in [46] can be modified such that $\mathcal{G} = T^*\mathbb{R}^n$ is equipped with the canonical symplectic structure. The source and target maps defined in [46] then become, with (x, p) cotangent coordinates on $T^*\mathbb{R}^n$:

$$\begin{cases} \alpha : (x,p) \mapsto \left(e^{-\frac{1}{2}\sum_i a_{ij} x_i p_i} . x_j \right)_{j=1,\dots,n} \\ \beta : (x,p) \mapsto \left(e^{\frac{1}{2}\sum_i a_{ij} x_i p_i} . x_j \right)_{j=1,\dots,n} \end{cases} \tag{3.40}$$

The triple $(T^*\mathbb{R}^n, \alpha, \beta)$ is a bi-realisation of the Poisson structure (3.39).

3.3.2 Lagrangian bi-sections and Hamilton-Jacobi equation

We are now ready to use bi-realisations in order to look for Poisson integrators that approximate the flow of a Hamiltonian H, by considering them as graphs of closed 1-forms on M.

More precisely, assume we are given $(\mathcal{U}, \alpha, \beta)$ a bi-realisation of a Poisson manifold (M, π) and H a Hamiltonian function. In the sequel, we will see from (3.41) that the flow of H corresponds to a family $(L_t)_{t\in I}$ of Lagrangian bi-sections of the symplectic groupoid $(\mathcal{G}, \Omega)$, with $L_0 = M$. Reducing I if necessary, the bi-sections $(L_t)_{t\in I}$ become Lagrangian submanifolds in an open subset $\mathcal{U}$ of (T^*M, ω_{can}). Since L_0 is the zero section, L_t is the graph of a closed 1-form $\zeta_t \in \mathcal{C}^\infty(M)$ depending smoothly on t. This form is exact, thanks to the following proposition. Local assumptions are set to make the statement precise.

Proposition 3.3.9. *Let $\xi \in \Omega^1_0(U)$, $U \subset M$ a relatively compact open subset and I a sufficiently small open interval containing* 0.

[3] $\mathfrak{g}^{**} \simeq \mathfrak{g}$

1. *There exists a unique smooth family of* 1*-forms* $(\zeta_t)_{t\in I}$ *such that their graphs have* ξ *as variation form:* $\bar{\zeta}_t = \Phi^t_{\overrightarrow{\xi}}(U)$.

2. *For all* t, ζ_t *is exact if and only if* ξ *is also exact.*

Proof. For I sufficiently small, the flow of $\overrightarrow{\xi}$ is complete. Furthermore, the map $\psi_t = \tau \circ \Phi^t_{\overrightarrow{\xi}}$ is a diffeomorphism of U for all $t \in I$. That allows to set $\zeta_t = \Phi^t_{\overrightarrow{\xi}}(\psi_t)^{-1}$ and to prove the first point.

Setting $L_t = \Phi^t_{\overrightarrow{\xi}}(U)$, the second point comes from example 3.2.23 and the bijectivity of τ and α when they are restricted to L_t: there exists $f \in \mathcal{C}^\infty(U)$ such that $\xi = \mathrm{d}f$ if and only if $\zeta_t = \mathrm{d}\int_0^t (\alpha \circ \tau^{-1}_{|L_s})^* f \mathrm{d}s$.. The other direction follows the same principle. □

Corollary 3.3.10. *When* $\xi = dH$ *is exact, the closed* 1*-forms* ζ_t *are exact:* $\zeta_t = dS_t$*, with* $(S_t)_t \in \mathcal{C}^\infty(U \times I)$ *a solution of*

$$\begin{cases} \partial_t S_t(m) & = (\tau_{|\underline{dS_t}})^{-1*} \alpha^*_{|\underline{dS_t}} H(m) + \chi(t) \\ S_0 & = 0 \end{cases}, \tag{3.41}$$

and where $\chi(t) \in \mathcal{C}^\infty(I, \mathbb{R})$ *is any smooth function and* τ *is the cotangent projection.*

Proof. From $\xi = \mathrm{d}H$, one deduces:

$$\frac{\mathrm{d}\zeta_t}{\mathrm{dt}} = \mathrm{d}(\alpha \circ \tau^{-1}_{|\zeta_t})^* H \tag{3.42}$$

and the exactness of ζ_t for all t: $\zeta_t = \mathrm{d}S_t$. To recover equation (3.41), observe that pull-backs are contravariant and integrate to get the desired equality of smooth functions. □

We call (3.41) the *Hamilton-Jacobi equation* for a Poisson structure. Since χ is arbitrary and plays no role, it will be set to 0.

Remark 3.3.11. Let us comment on the initial condition $S_0 = 0$. In the context of this chapter, we are mainly interested with local embeddings of the symplectic groupoid $\mathcal{G}$ in some cotangent bundle T^*V such that the unit space M coincides with the base V. It may happen, though, that one considers embeddings where this property does not hold. For instance, the symplectic groupoid T^*G of the dual of an integrable Lie algebroid $A = \mathrm{Lie}(G)$ is naturally fibered on its groupoid G but the fibration is transverse to the unit space. In those cases, it still makes sense to look for Lagrangian bi-sections as graphs of closed forms, but only if they are sufficiently far from M. There, one might relax the condition $S_0 = 0$ and build a family of Poisson automorphisms that are no perturbation of the identity map.

Remark 3.3.12. For a linear Poisson structure, [27] explains how to obtain numerical methods preserving the Lie-Poisson structure. This framework is then developped for a general setting in [26] to obtain a coordinate version of (3.41).

Theorem 3.3.13. *Assume we are given* $(\mathcal{U}, \alpha, \beta)$ *a bi-realisation of a Poisson manifold* (M, π) *and* H *a Hamiltonian function.*

1. *The Hamilton-Jacobi equation* (3.41) *admits a solution* $(S_t)_t$ *in a neighborhood of* $M \times \{0\} \subset M \times \mathbb{R}$.

2. *The family of Poisson automorphisms induced by the Lagrangian bi-sections* $(dS_t)_t$ *is the flow of* H.

Proof. The embedding of $\mathcal{G} \rightrightarrows M$ in T^*M allows to express Lagrangian bi-sections near the base with graphs of closed 1-forms in a smooth way. That explains the first point.

Similar computation as example 3.2.23 gives the Hamiltonian H induced by $(dS_t)_t$, which admits the differential:

$$(\alpha^{-1}_{|\underline{dS_t}})^* {\tau_{|\underline{dS_t}}}^* d\partial_t S_t = dH.$$

□

Remark 3.3.14. Let us relate the usual Hamilton-Jacobi equation described in Section 3.2.2 with the equation we present in this section.

For the first one: $\Phi^t_{\overrightarrow{H}}(T^*Q) \subset T^*Q \times T^*Q$ is related by some graph of exact one-form dS_t on $Q \times Q$ by Ψ defined in (3.14).

For the second one: $\Phi^t_{\overrightarrow{H}}(M) \subset \mathcal{G}$ is related by some graph of exact one-form dS_t on M by the bi-realisation.

Equation (3.41) is analogous to equation (3.17) and its generalizations in [23] in the sense of variations of Lagrangian bi-sections. Indeed, the equation (3.17) measures Lagrangian perturbations of the diagonal in $T^*Q \times T^*Q$ by 1-forms on $Q \times Q$ through the canonical symplectomorphism (3.14) while the second one measures Lagrangian perturbations of M in its local symplectic groupoid by 1-forms on M through some bi-realisation.

3.3.3 Main result and construction of the Hamiltonian Poisson integrators

The computation of $(S_t)_t$ is not of interest from a numerical aspect because it is equivalent to integrate the Hamiltonian flow. Nevertheless, a natural consequence of theorem 3.3.13 is that the first terms of the expansion of $(S_t)_t$ with respect to t induce an approximation of similar order of the flow of H.

Theorem 3.3.15. *Assume we are given $(\mathcal{U}, \alpha, \beta)$ a bi-realisation of a Poisson manifold (M, π) and H an Hamiltonian function. Define recursively a family $(S_i)_{i\in\mathbb{N}}$ of smooth functions on M by $S_0 = 0$, $S_1 = H$, $S_2(m) = \frac{d}{dt}|_{t=0} H(\alpha(td_mH))$, and*

$$S_{i+1}(m) = \left.\frac{d^i}{dt^i}\right|_{t=0} H\left(\alpha\left(d_m S_t^{(i)}\right)\right) \tag{3.43}$$

where $S_t^{(i)} = \sum_{j=1}^{i} \frac{t^j}{j!} S_j$.

The family of Poisson automorphisms associated to the Lagrangian bi-sections $d\left(S_t^{(k)}\right)$ are Hamiltonian Poisson integrators of order k for H with variation functions :

$$dh_t = (\tau_{|\underline{dS_t^{(k)}}} \circ \alpha^{-1}_{|\underline{dS_t^{(k)}}})^* d\partial_t S_t^{(k)} \tag{3.44}$$

and the modified Hamiltonian verifies $\mathcal{M}_\epsilon(h) = \epsilon H + o\left(\epsilon^k\right)$.

Remark 3.3.16. The term of S_t of order 1 in t is necessarily H.

Remark 3.3.17. $S_t = \sum_{i=1}^{\infty} \frac{1}{i!} S_i$ is a solution of the formal Hamilton-Jacobi equation, i.e. equation (3.41) made formal in t and $S_t^{(k)}$ is the truncation at order k or this solution.

Our general algorithm of a Poisson integrator of timestep Δt for H at order k, following remark 3.2.17 and theorem 3.3.15, is given by the three steps:

1. Use recursion (3.43) to compute the k-th terms of $(S_t^{(k)})_t$.

2. starting from $x \in M$, solve

$$x = \alpha(d_{\overline{x}} S^{(k)}_{\Delta t}),\ \overline{x} \in M, \tag{3.45}$$

3. and project

$$\tilde{x} = \beta(d_{\overline{x}} S^{(k)}_{\Delta t}). \tag{3.46}$$

It is clear that near any point $x \in M$ and for small Δt, equation (3.45) always has a solution.

This extends definition 2.1.10 to Poisson manifolds. We have completed the task of associating to any bi-realisation and any Hamiltonian H a Hamiltonian Poisson integrator of arbitrary order and time-step.

3.3.4 An algebraic formula for the formal Hamilton-Jacobi equation

In section 2.5.1, we have explained how to construct a solution of the formal Hamilton-Jacobi equation. We repeat it here quasi-verbatim, but for a generic manifold M. We will not recall some examples and first terms given in section 2.5.1.

Let $\mathcal{P}_n$ be the list of all ordered tuples $(p_1, \dots, p_k)$ of non-zero positive integers such that $p_1 + \cdots + p_k = n$, i.e. partitions of n. We warn the reader that, for us, $(1,3)$ and $(3,1)$ are different partitions of 4. To any $(p_1, \dots, p_k) \in \mathcal{P}_n$, we now associate an integer $\beta(p_1, \dots, p_k)$ as follows. Define $\mathcal{S}$ as the free $\mathbb{N}$ module generated by polynomials with coefficients in $\mathbb{H}$. In short,

$$\mathcal{S} = \mathbb{N}\Big[\mathbb{N}[X]\Big]$$

We denote elements of $\mathcal{S}$ by $\sum_i n_i \diamond \left\{ P_i \right\}$ with $n_i \in \mathbb{N}$ and $P_i \in \mathbb{N}[X]$. Again, we warn the reader not to confuse $3 \diamond \left\{ 2X + X^2 \right\}$ with $\left\{ 6X + 3X^2 \right\}$: those are different elements in $\mathcal{S}$.

We now define a $\mathbb{N}$-linear endomorphism of $\mathcal{S}$ which is given for any polynomial $P \in \mathbb{N}[X]$ of degree $|P|$ by:

$$\begin{array}{rcl} I : \mathcal{S} & \longrightarrow & \mathcal{S} \\ P & \longmapsto & \sum_{i=1}^{|P|+1} \left\{ P + X^j \right\} \end{array}$$

Definition 3.3.18 (Farmer sequence)**.** Define the sequence $(\mathcal{A}_n)_{n \geqslant 1}$ valued in $\mathcal{S}$ as the iterations of I starting at $\left\{ X \right\}$:

$$\left\{ \begin{array}{rcl} \mathcal{A}_1 = & \left\{ X \right\} \\ \mathcal{A}_{n+1} = & I(\mathcal{A}_n) \end{array} \right. \tag{3.47}$$

It is routine to check that $\mathcal{A}_n$ is a linear combination of polynomials P such that $P(1) = n$ and of the form $\sum_{i=1}^{k} p_i X^i$ where none of the integral coefficients $p_1, \ldots, p_k$ are zero. As a consequence, it is of the form

$$\mathcal{A}_n = \sum_{(p_1,\ldots,p_k)\in\mathcal{P}_n} \beta(p_1,\ldots,p_k) \diamond \left\{ p_1 X + \cdots + p_k X^k \right\}$$

for some integers $\beta(p_1, \ldots, p_k)$. The following definition now makes sense:

Definition 3.3.19. Consider a bi-realisation with source α, target β and projection $\tau : \mathcal{W} \to \mathcal{U}$. To any Hamiltonian $H \in \mathcal{C}^\infty(M)$, we associate a formal power series $S_H := \sum_{i=1}^{\infty} \frac{t^i}{i!} S_i$ in $\mathcal{C}^\infty(M)[[t]]$ where the sequence $(S_n)_{n\geqslant 1}$ is defined recursively by $S_1 = H$, and:

$$S_{n+1} = \sum_{(p_1,\ldots,p_k)\in\mathcal{P}_n} \beta(p_1,\ldots,p_k)\ \mathbf{0}^* \left(\mathrm{ad}_{\tau^* S_{p_k}} \ldots \mathrm{ad}_{\tau^* S_{p_1}} \alpha^* H \right).$$

where $\mathrm{ad}_g f = \{f, g\}$ is the adjoint action of the canonical Poisson bracket on $\mathcal{C}^\infty(T^*M)$ and $\mathbf{0}\colon M \to T^*M$ is the zero section of the vector bundle $\tau\colon T^*M \to M$.

We need the following lemma in order to state the main result.

Lemma 3.3.20. *For all $F \in \mathcal{C}^\infty(T^*M \times I)$ and $G \in \mathcal{C}^\infty(M \times I)$,*

$$\frac{d}{dt}(dG_t)^* F_t = (dG_t)^* \left(\frac{dF_t}{dt} + \left\{ F_t, \tau^* \frac{dG_t}{dt} \right\} \right), \tag{3.48}$$

where $\{.,.\}$ is the Poisson bracket of the canonical symplectic form and $(dG_t)^*$ denotes the pull-back by the section $m \in M \mapsto d_m G_t \in T^*M$.

Proof. From the chain rule:

$$\frac{\mathrm{d}}{\mathrm{dt}}(\mathrm{d}G_t)^* F_t = (\mathrm{d}G_t)^* \left(\frac{\mathrm{d}F_t}{\mathrm{dt}} + \left\langle \mathrm{d}F_t, \mathrm{d}\frac{\mathrm{d}G_t}{\mathrm{dt}} \right\rangle \right),$$

where $\mathrm{d}\frac{\mathrm{d}G_t}{\mathrm{dt}}$ is the vector field on T^*M having fibers preserving integral curves

$$(t, p) \in \mathbb{R} \times T^*M \mapsto p + t\mathrm{d}_{\tau(p)} \frac{\mathrm{d}G_t}{\mathrm{dt}}.$$

In order to conclude, we are left to prove that this is the Hamiltonian vector field of $\tau^* \frac{\mathrm{d}G_t}{\mathrm{dt}}$. This holds thanks to the construction of the canonical symplectic form. □

Remark 3.3.21. In what follows, this lemma will be applied repeatedly to get more derivative formulae. For instance:

$$\begin{aligned} \frac{\mathrm{d}^2}{\mathrm{dt}^2}(\mathrm{d}G_t)^* F_t =& (\mathrm{d}G_t)^* \left(\frac{\mathrm{d}^2 F_t}{\mathrm{dt}^2} + 2\left\{ \frac{\mathrm{d}F_t}{\mathrm{dt}}, \tau^* \frac{\mathrm{d}G_t}{\mathrm{dt}} \right\} + \left\{ F_t, \tau^* \frac{\mathrm{d}^2 G_t}{\mathrm{dt}^2} \right\} \right. \\ &\left. + \left\{ \left\{ F_t, \tau^* \frac{\mathrm{d}G_t}{\mathrm{dt}} \right\}, \tau^* \frac{\mathrm{d}G_t}{\mathrm{dt}} \right\} \right) \end{aligned} \tag{3.49}$$

Notice that each term of the previous sum is either a second derivative or some Poisson brackets iterated k times, the i-th of them being a n_i-th derivative with $\sum_{i=1}^{k} n_i = 2$. Roughly speaking, each term has 2 "$\frac{\mathrm{d}}{\mathrm{dt}}$". In general, "$\frac{\mathrm{d}^j}{\mathrm{dt}^j}(\mathrm{d}G_t)^* F_t$" is a sum of terms that all contain j "$\frac{\mathrm{d}}{\mathrm{dt}}$". This fact underlies the appearance of the β coefficents in the next theorem.

Here is the main result, describing the solution of the formal Hamilton-Jacobi equation.

Theorem 3.3.22. *For any Hamiltonian function H on (M,π), and for any bi-realisation $(\mathcal{W},\alpha,\beta)$, the formal function $S_t = \sum_{i=1}^{\infty} \frac{t^i}{i!} S_i \in \mathcal{C}^\infty(\mathcal{U})[[t]]$ is the solution of the formal Hamilton-Jacobi equation* (3.43) *(i.e. is the formal Hamilton-Jacobi transform of the Hamiltonian H) if and only if S verifies definition 3.3.19.*

Also, for every $k \geqslant 1$, the function $S_t^{(k)} := \sum_{i=1}^{k} \frac{t^i}{i!} S_i$ is a solution of the formal Hamilton-Jacobi equation up to order k.

Proof. The proof is based on a repeated use of lemma 3.3.20. Let $S_t = \sum_{i=1}^{\infty} \frac{t^i}{i!} S_i \in \mathcal{C}^\infty(\mathcal{U})[[t]]$ be the solution of the formal Hamilton-Jacobi equation (3.43), $j \geqslant 2$ and let us show that

$$S_{j+1} = \sum_{(p_1,\dots,p_k)\in\mathcal{P}_j} \beta(p_1,\dots,p_k)\ \mathbf{0}^*\left(\mathrm{ad}_{\tau^* S_{p_k}} \dots \mathrm{ad}_{\tau^* S_{p_1}} \alpha^* H\right). \tag{3.50}$$

For any $l \in [\![1, j]\!]$, lemma 3.3.20 applied l times to $\alpha^* H(\mathrm{d}S_t)$ gives

$$\frac{\mathrm{d}^j}{\mathrm{d}t^j}(\mathrm{d}S_t)^*\alpha^* H = \frac{\mathrm{d}^{j-l}}{\mathrm{d}t^{j-l}}(\mathrm{d}S_t)^* \sum_{(p_1,\dots,p_k)\in\mathcal{P}_l} \beta(p_1,\dots,p_k)\ \mathbf{0}^*\left(\mathrm{ad}_{\tau^*\frac{\mathrm{d}^{p_k} S_t}{\mathrm{d}t^{p_k}}} \dots \mathrm{ad}_{\tau^*\frac{\mathrm{d}^{p_1} S_t}{\mathrm{d}t^{p_1}}} \alpha^* H\right). \tag{3.51}$$

The result follows by setting $l = j$ and $t = 0$.

□

Conclusion

Let us sum up the message of this chapter. A bi-realisation of a Poisson manifold M, or equivalently a symplectomorphism between the local symplectic groupoid and a neighborhood of the base in T^*M, allows to transform, through the analog of the Hamilton-Jacobi equation, a Hamiltonian $H \in \mathcal{C}^\infty(M)$ into a smooth family of functions $(S_t)_t$ on M with $S_0 = 0$. Then, using the induced Lagrangian bi-sections $\underline{(\mathrm{d}S_t)_t}$, the source and the target, the recursively computed truncation $S^{(k)}$ of order k of S gives a Poisson integrator $\phi_{\Delta t} = \beta \circ (\alpha_{\underline{dS^{(k)}_{\Delta t}}})^{-1}$ of order k for H. These integrators have strong geometric properties: not only their iterations stay on the symplectic leaf of the initial point (even a singular one), but they also follow the exact flow of a Hamiltonian on the manifold, which coincides with H up to order $k-1$.

Hence the groupoid formalism developed in section 3.2 proved to be useful for the construction of integrators. As one could expect, most existing Poisson integrators were already of that form, although not understood as such. Moreover, the Magnus formula introduced in section 3.1 gives a new constructive way to compute the modified Hamiltonian of a Hamiltonian Poisson scheme and a new point of view on backward analysis in the context of geometric integrators for symplectic and Poisson geometry.

As mentioned in the introduction, one expects those integrators to be of particular interest in mechanics, where it matters to preserve properties of the dynamics when discretizing trajectories. In order to illustrate the link between their geometric properties and their long-term stability, we implement and benchmark some Poisson schemes of section 3.3.3 in the next chapter, to study them from a numerical aspect in comparison with other classical and geometric methods available to the

community. A more "applied" reader may have skipped the above purely mathematical chapter, some "minimal working knowledge" in geometry being reviewed in chapter 2, obviously at the expence of proofs and generalizations. See also [15]. We will now apply those constructions to problems from mechanics.

CHAPTER 4

Numerical Methods in Poisson Geometry and Applications in Mechanics

based on arXiv:2303.15883

We give in this chapter numerical experimentations to test the Hamiltonian Poisson integrators that we have introduced in definition 2.4.5 and are at the heart of this work. Since it is devoted to applications, let us give a non-exhaustive list. Poisson geometry allows to describe a large class of conservative systems in mechanics, both for discrete and continuous media. Those may be obtained as a result of a reduction procedure or as an ad hoc model for evolution of some natural systems. To cite a few: chemistry (polymer dynamics, [25]), plasticity (elastoplasticity, [49]), population dynamics ([41, 21]), liquid crystals theory ([24]), thermodynamics (GENERIC formalism, [31]), control theory (active and kinematic constraints, [53]).

In all those examples, the Poisson structure matters to express symmetries, conservation laws and qualitative behaviour of the considered dynamical system. We illustrate in this chapter the importance of preserving those features during numerical computations.

4.1 Non-Hamiltonian Poisson integrators

Important examples of Poisson structures are the symplectic ones in their canonical form, e.g. where $\pi = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix}$. For those, a wide example of symplectic integrators are already available in the literature. One construction of such integrators uses the principle of symplectic Runge–Kutta schemes ([75]):

$$\begin{aligned} x_{n+1} &= x_n + \Delta t \sum_{i=1}^{s} b_i k_i \\ k_i &= \pi(x_n + \Delta t \sum_{j=1}^{n} a_{ij} k_j) \cdot \nabla H(x_n + \Delta t \sum_{j=1}^{n} a_{ij} k_j) \end{aligned} \tag{4.1}$$

where slopes k_i are implicitly defined and coefficients b_i and a_{ij} are chosen such that the discrete flow preserves π. For this precise π, any trajectory preserving it is necessary a time-dependent Hamiltonian one, at least locally.

For a Poisson structure π on a vector space given by a constant but degenerate skew-symmetric matrix, the same principle can be applied ([36]) and leads to a discrete flow that preserves the Poisson tensor, i.e. a Poisson integrator. However, it may lead to non-physical simulations, e.g. non-Hamiltonian Poisson integrators. It does not guarantee the Hamiltonian property of the discrete trajectory anymore because of the existence of outer Poisson automorphisms, as illustrated in the following example.

Example 4.1.1. Consider $\mathcal{U} = \mathbb{R}^3$. The system of differential equations

$$\begin{cases} \dot{x} &= -\frac{(x+y-z)}{8}\left((-x-y+z)^2 + (x+y-z)^2\right) \\ \dot{y} &= \frac{(-y+z)}{4}\left((x-y+z)^2 + (x+y-z)^2\right) \\ \dot{z} &= \frac{(x-y+z)}{8}\left((x-y+z)^2 + (x+y-z)^2\right) \end{cases} \tag{4.2}$$

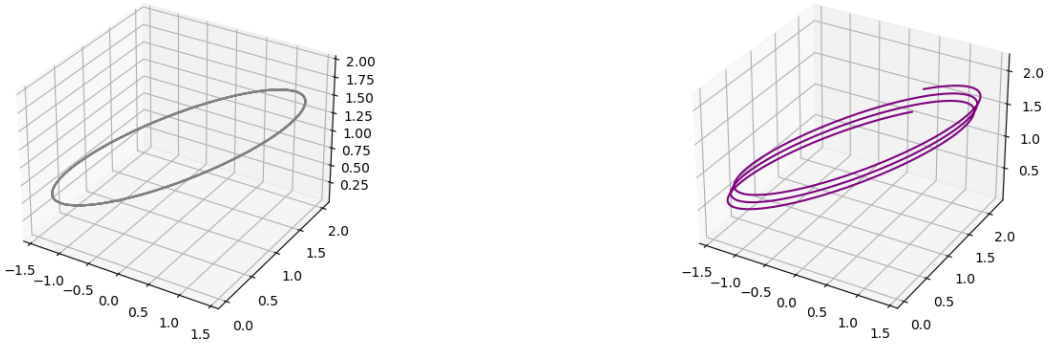
is Hamiltonian with respect to the Poisson structure

$$\pi(x,y,z) = \frac{(x-y+z)^2 + (x+y-z)^2}{4} \begin{pmatrix} 0 & -1 & -1 \\ 1 & 0 & -1 \\ 1 & 1 & 0 \end{pmatrix}$$

and the Hamiltonian $H\colon (x,y,z) \mapsto \frac{(x-y+z)^2+(x+y-z)^2}{8}$. For any $\Delta t > 0$, the system of equations:

$$\begin{cases} x_{n+1} = & x_n \cos\left(\Delta t \frac{x_n^2+y_n^2-2y_nz_n+z_n^2}{2}\right) + y_n \sin\left(\Delta t \frac{x_n^2+y_n^2-2y_nz_n+z_n^2}{2}\right) \\ & -z_n \sin\left(\Delta t \frac{x_n^2+y_n^2-2y_nz_n+z_n^2}{2}\right) \\ y_{n+1} = & \frac{-x_n+y_n-z_n}{2} \sin\left(\Delta t \frac{(x_n-y_n+z_n)^2+(x_n+y_n-z_n)^2}{4}\right) + \frac{-x_n+y_n+z_n}{2} \exp\left(\Delta t^k\right) \\ & + \frac{x_n+y_n-z_n}{2} \cos\left(\Delta t \frac{(x_n-y_n+z_n)^2+(x_n+y_n-z_n)^2}{4}\right) \\ z_{n+1} = & \frac{-x_n+y_n+z_n}{2} \exp\left(\Delta t^k\right) + \frac{x_n-y_n+z_n}{2} \cos\left(\Delta t \frac{(x_n-y_n+z_n)^2+(x_n+y_n-z_n)^2}{4}\right) \\ & + \frac{x_n+y_n-z_n}{2} \sin\left(\Delta t \frac{(x_n-y_n+z_n)^2+(x_n+y_n-z_n)^2}{4}\right) \end{cases} \tag{4.3}$$

is a discretisation of order k of the differential equation (4.2). A direct computation shows that it is a Poisson integrator, i.e. $(x_n, y_n, z_n) \mapsto (x_{n+1}, y_{n+1}, z_{n+1})$ is a Poisson isomorphism. However, it is *not* a Hamiltonian Poisson integrator. This can be proven as follows: for any vector field on $\mathbb{R}^3$ that vanishes at least quadratically at $(0,0,0)$, the differential of its flow at $(0,0,0)$ is the identity map. In particular, since the coefficients of the Poisson structure vanish at least quadratically at $(0,0,0)$, so does any Hamiltonian vector field, so that any Hamiltonian Poisson integrator should be made of a local diffeomorphism whose differential at $(0,0,0)$ is the identity map. Since the differential at $(0,0,0)$ of the map $(x_n, y_n, z_n) \mapsto (x_{n+1}, y_{n+1}, z_{n+1})$ is not equal to identity map, the latter Poisson integrator is not Hamiltonian.



(a) Flow of (4.2)

(b) Poisson integrator (4.3)

Figure 4.1: Discrepancy created by the Poisson integrator (4.3)

Figures 4.1.A and 4.1.B show the difference between the actual flow of (4.2) and the first iterations of the Poisson integrator (4.3) at order $k = 2$ with initial points $\begin{pmatrix} 1 \\ 1 \\ 2 \end{pmatrix}$ and timestep $\Delta t = 10^{-4}$. The flow should be 4π-periodic while an approximation of it at order 2 destroys the topology of the curve, even while it preserves the Poisson tensor. The geometric reason is that the Poisson integrator (4.3) does not stay on a symplectic leaf of the Poisson structure, i.e. a hyperplane of equation $\{x - y + z = \text{constant}\}$.

In conclusion, non-Hamiltonian Poisson integrator may have long term behaviour that is extremely un-natural and non-physical.

4.2 Numerical tests for Hamiltonian Poisson integrators

In this section we illustrate the advantages of our Hamiltonian Poisson integrators coming from explicit bi-realisations on a couple of examples. This is based on two natural examples of those described in section 2.2.3: a linear one and a quadratic one.

4.2.1 The Rigid Body

First turn to the linear Poisson structures and to the dynamics of a rigid body about a periodic orbit.

The equations governing the system read:

$$\dot{x} = -x \wedge J.x,$$

where $\wedge$ denotes the vector product in $\mathbb{R}^3$, and the symmetric positive matrix J is the inertia tensor of the body. It is a Hamiltonian differential equation for $\pi(x) = \begin{pmatrix} 0 & -x_3 & x_2 \\ x_3 & 0 & -x_1 \\ -x_2 & x_1 & 0 \end{pmatrix}$ and $H(x) = \frac{1}{2}\mathrm{Tr}\Big(j(x)^T.J.j(x)\Big)$ where $j\colon \mathbb{R}^3 \tilde{\longrightarrow} so(3)$ given by:

$$x \longmapsto \begin{pmatrix} 0 & -x_3 & x_2 \\ x_3 & 0 & x_1 \\ -x_2 & -x_1 & 0 \end{pmatrix}.$$

This can be reinterpreted as being an Hamiltonian differential equation on teh dual of $so(3)$, equipped with its canonical Poisson structure.

For our numerical example, we consider the inertia tensor $J = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \pi & 0 \\ 0 & 0 & 100 \end{pmatrix}$ and $x_0 = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$ The trajectory is in this case given by Figure 4.2. It is a periodic trajectory: this is expected since we work in dimension 3 and since the Casimir function (=the square of the norm) and H has to be preserved, which imposes that most integral curves are in fact loops.

We apply our method:

1. to the bi-realization of the linear Poisson structure on the dual of $so(3)$ obtained using the Cayley transform, i.e. the local diffomorphism $so(3) \to SO(3)$ described in (2.14):

$$\varphi\colon SO(3)_+ \to so(3) : Q \mapsto 4\frac{Q-I}{Q+I}$$

2. at order 2

3. the initial point above and $\Delta t = 10^{-4}$.

We call HPI-2 the henceforth obtained Hamiltonian Poisson integrator.

We will test:

- if the symplectic leaves are preserved, i.e. if the concentric spheres are preserved, i.e. if the square of the norm is preserved, and
- if the Hamiltonian function H is preserved.

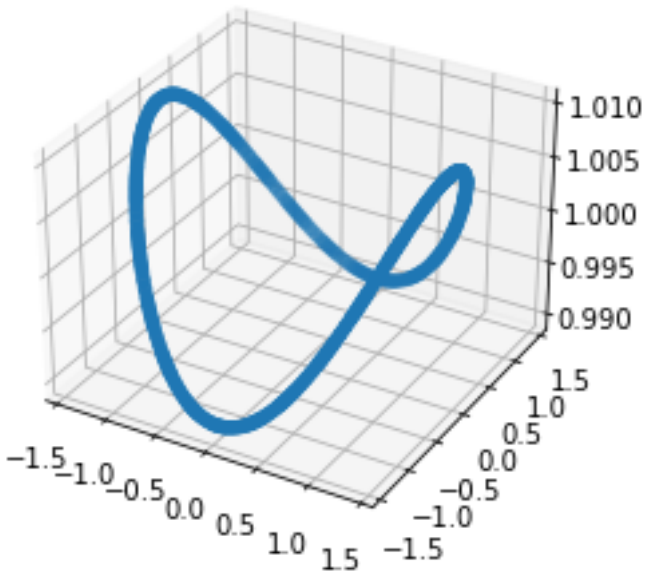


Figure 4.2: The trajectory of the angular velocity of a rigid body in $\mathbb{R}^3$.

In dimension 3, preserving these two functions tells if the integrator makes sense or not.

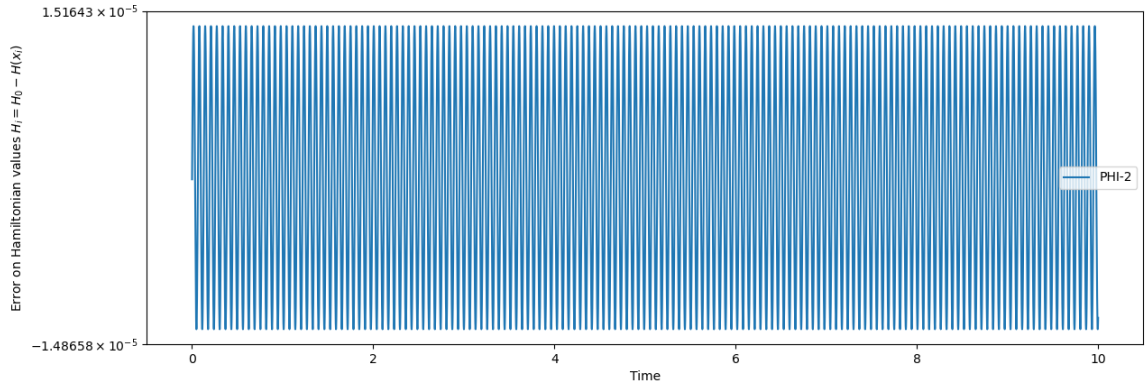
HPI-2 behaves much better than the Runge-Kutta method of order 4 in the preservation of both Casimir and Hamiltonian levels (Figure 4.3).

The Hamiltonian Poisson integrator (HPI-2) preserves the level of the Casimir functions at machine precision. The error of the traditional method (RK-4) depends linearly on the number of iterations and so diverges from the continuous (closed) trajectory. In Figure 4.3 we have plotted only the first 10 time units of integration to stress these two phenomena.

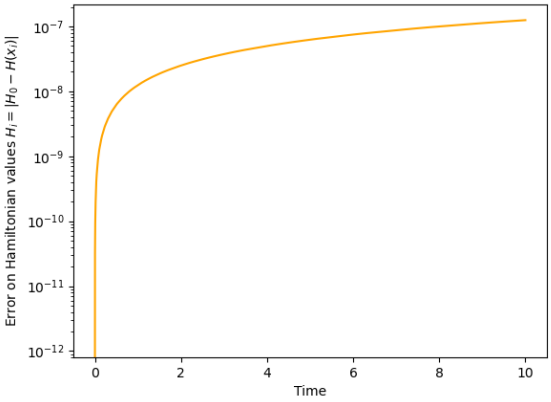
Also, HPI-2 oscillates around a Hamiltonian value with an amplitude depending on Δt. Although RK-4 has a better precision, we emphasize that in a longer simulation the amplitude of oscillations for the HPI-2 integrator *does not* increase, while for RK-4 the linear growth is still observed. Hence, one recovers a typical stability phenomenon of symplectic integrators, already noticed and explained in [5].

Remark 4.2.1. The Casimir in this case is the square of the norm. Hence Figure 4.3c indicates that RK-4 iterations will converge to 0 in $\mathbb{R}^3$, which is a fixed point of the dynamics as well as a singular leaf of the foliation of the total space. This lead on long run simulations to pathological behaviours. In turn, it stresses the importance of numerical methods preserving leaves of a singular foliation such as the ones appearing in Poisson structures.

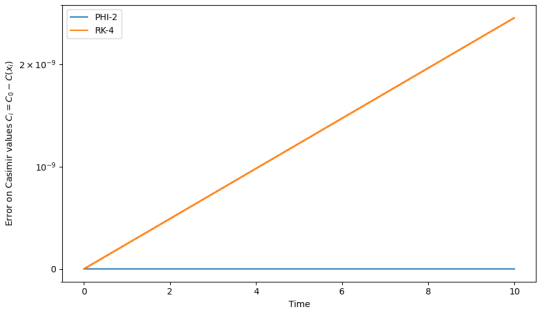
The theoretical explanations relies on the Magnus formula for the Poisson structures introduced in section 2.5.2. For the convenience of the reader, the schematic sections of the trajectory and their integrators are illustrated on Figure 4.4.



(a) Errors on Hamiltonian values for HPI-2

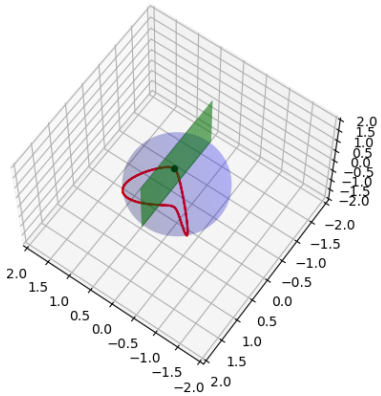


(b) Errors on Hamiltonian values for RK-4

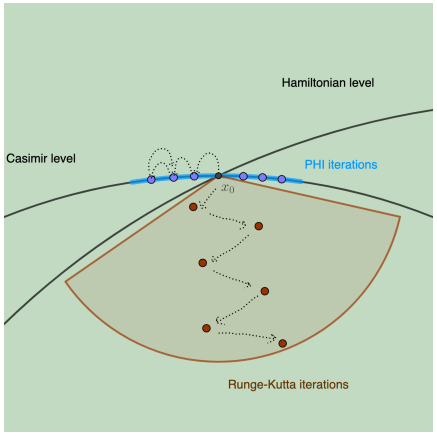


(c) Error on Casimir values for HPI-2 and RK-4

Figure 4.3: Comparison between Runge-Kutta 4 and our Hamiltonian Poisson integrator at order 2 for the Rigid Body dynamics



(a) A Poincaré section of the trajectory (green plane)



(b) Intersection between (interpolated) discrete trajectories and the Poincaré section

Figure 4.4: Illustration "drawn by hand" of the difference of behaviour of two numerical methods with respect to Hamiltonian and Casimir levels

4.2.2 The Lotka-Volterra System

Let us look at a particular case of Lotka-Volterra type equations

$$\begin{aligned}\dot{x}_1 &= x_1(x_2 + x_3)\\ \dot{x}_2 &= x_2(-x_1 + x_3)\\ \dot{x}_3 &= -x_3(x_1 + x_2).\end{aligned}$$

This system of differential equations appears in [72] (page 97, equation (16)) as a model in population dynamics, and similar systems have been extensively studied since then (e.g. [21]). For this particular one, an explicit solution was computed in [41]: it allows to compare, for any initial point and desired time, numerical simulations with the exact solution $x^{\text{exact}}(t) = (x_1(t), x_2(t), x_3(t))$.
Some integral curves $x^{\text{exact}}(t)$ go to infinity, exploding exponentially fast while approaching some specific time. For instance, using the exact formulas given in [41], one observes that for the initial value

$$\begin{pmatrix} x_1(0)\\ x_2(0)\\ x_3(0)\end{pmatrix} = \begin{pmatrix} -3\\ 5\\ 10^{-3}\end{pmatrix},$$

the trajectory $x^{\text{exact}}(t)$ starts exploding around $T_{sing} \simeq 0.23$. We use this singularity to test the standard explicit 2nd order Runge–Kutta method (RK-2) and a Hamiltonian Poisson integrator of order 1 (HPI-1).

In short, we apply our method:

1. to the Poisson structure of the generic Lotka-Volterra system is the quadratic Poisson structure of Equation (2.12) encoded by the 3×3 matrix
$$A = \begin{pmatrix} 0 & 1 & 1\\ -1 & 0 & 1\\ -1 & -1 & 0\end{pmatrix},$$
2. to the explicit bi-realization explained in equation (2.13),
3. at order 1,
4. for the dynamics is governed by the linear Hamiltonian $H = x_1 + x_2 + x_3$,
5. and the initial value
$$\begin{pmatrix} -3\\ 5\\ 10^{-3}\end{pmatrix}.$$

Since there exists an explicit expression of the solution, we will simply compare our numerical integrators to that explicit solution. It is also interesting to see how much they preserve a local Casimir functions, which, in our case in the function: $C\colon x \mapsto \frac{x_1 x_3}{x_2}$.

Remark 4.2.2. For the quadratic structure described in Equation (2.12) out of a generic skew-symmetric matrix A, for every $u \in \mathrm{Ker} A$.

$$\begin{aligned} f\colon {\mathbb{R}_+}^n &\to \mathbb{R}\\ x &\mapsto \prod_{1\leqslant i\leqslant n} x_i^{u_i}\end{aligned}$$

is a local Casimir function. Hence the expression of the Casimir in the case we are interested in.

Here is what numerical simulations show: although our Hamiltonian Poisson integrator is of order 1 only, it performs much better than the order two Runge-Kutta method near the singularity T_{sing} described above (see Fig. 4.5):

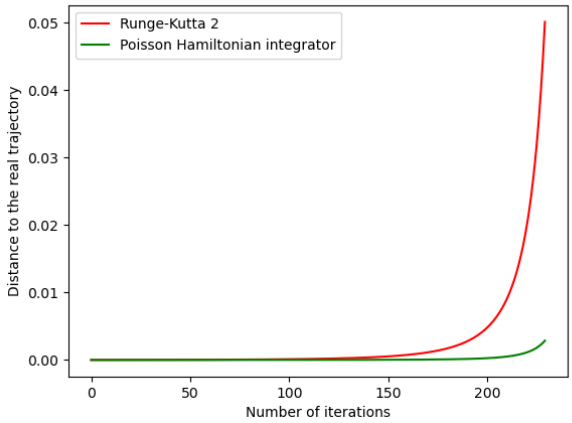


Figure 4.5: Comparison of the error for RK-2 and HPI-1: the sigularity is around 223

We observe that the HPI-1 method approximates the solution much better than the RK-2. In fact comparing the values of the variables, we see that the RK-2 misses the singularity completely, in a sense that it goes off the exact solution much earlier than it may tend to infinity, so using it alone one would not even notice that the solution is singular; while the HPI-1 method pushes the solution up to the last step before hitting the singularity, where it goes to what one can call "numerical infinity".

Also, the RK-2 Runge-Kutta method does not preserve C, while the constructed Hamiltonian Poisson integrator HP-1 does preserve the Casimir value with machine precision, see Figure 4.6 enlightens the stability of a Hamiltonian Poisson integrator in the neighborhood of a singularity observed on figure 4.5: on top of preserving the Poisson structure, it stays on a symplectic leaf along iterations, even near the singularity (which is around 0.23 the the previosu graph).

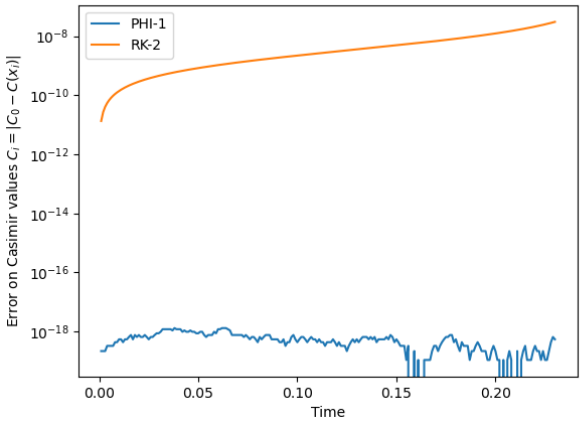


Figure 4.6: Comparison on Casimir values between HPI-1 and RK-2

It is actually quite unexpected that an order 1 integrator behaves better than an order 2 integrator. This example is especially interesting because we are in presence of a singularity. The explanation is

that as often in such a singular situation, an integrator that does not preserve the underlying geometric structure of the differential equations can not "see" the singulariy as well as an integrator that does preserve it.

Conclusion / perspectives

In this chapter, we have briefly explained how the idea of the groupoid construction from 3 was implemented for design of Poisson integrators. For some details once again we refer to [15]. Let us stress again that the term *Hamiltonian Poisson integrators* we have introduced is important – it explains the conceptual difference to constructions present in literature.

We have seen that even for simple academic examples constructed Hamiltonian Poisson integrators proved to be more accurate than even higher order classical methods, especially on long run simulations. But a similar strategy can be implemented with no changes for more complicated systems of ordinary differential equations – we are working on a symbolic package for automatic generation of the simulation source codes for that ([14]). Moreover, similar methods can be designed even for Poisson Hamiltonian partial differential equations, which often appear in fluid dynamics and waves simulations. The key idea there is to use the locality of discretisation in space to spell-out the groupoid structure maps – we intend to explore this direction in further works.

CHAPTER 5

On Dirac Structures Admitting a Variational Approach

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This more or less independent project on Dirac dynamics is ongoing. The approach is similar as the previous chapters: we hope that a better understanding of the geometric objects involved in the dynamics of a mechanical system will help to build robust numerical methods for this system. Previous chapters were dealing with Poisson Hamiltonian systems while in the following, Dirac Hamiltonian systems are dealt with. Apart from the philosophy of the approach, clear relations with the rest of the thesis are left to be done, as well as numerical applications. Therefore, we decided to present it apart from the main results of the present manuscript.

Introduction and motivation

Dirac structures, initially motivated by mechanics, have been first studied in a geometric framework ([17]) as a construction unifying symplectic geometry, Poisson structures and foliations altogether. Some port-Hamiltonian ([64]) and constrained systems ([76, 60]) can be mentioned as direct mechanical occurences of such structures. Dirac structures are also used as target spaces for gauge theories and describe – in a precise meaning – symmetry algebras of most general 2 dimensional sigma-models ([40]). In most of those works, the appearing Dirac structure is a consequence of the form of observables or of the gauge fields. In the present work, the question is somehow opposite.

The precise one we ask ourselves in this chapter can be vaguely formulated as: "given a Dirac structure, what else do we need to know to define meaningful dynamics on it". The question is in the spirit of [3], where the notion of *Dirac systems* is described in the context of constrains as well as for control theory; it also somehow complements the series of works [29, 30] on a uniform description, using algebroids, of constraint systems in both Hamiltonian and Lagrangian formalisms. All those works, like many others are inspired by the approach to mechanics using double vector bundles introduced in [66, 67]. In this chapter, more precisely, we study the cohomological conditions for a system arising from a Dirac structure to admit a variational (Lagrangian) formulation. For convenience, by some language abuse, we will call them *obstructions*, but what we actually mean is *sufficient conditions*. That is for "good cases", when this obstruction is absent, we explain how a Lagrangian is constructed. This includes some classes of Poisson structures, for which a variational formulation of Hamiltonian mechanics becomes possible. This is also an important step to the construction of Dirac structure-preserving numerical methods, since having constructed the Lagrangian, under some assumptions, one can profit from the well-established machinery of variational numerical methods.

The chapter is organized as follows. We start by recalling some notions of Lie algebroids we give the definition of their cohomology and describe the main geometric tool – cohomology of Dirac structures, providing some examples. We also explain the relation of this Dirac cohomology and the obstructions to construct a variational formulation for the dynamics on the Dirac structures. We illustrate the construction on some examples and counter-examples. To conclude, we explain some ideas about variational integrators and possible application of those in our setting – this is a separate rich topic that we intend to elaborate in another more "mechanically oriented" work.

5.1 The horizontal cohomology of Lie algebroids and Dirac structures

5.1.1 Lie algebroids

The notion of Lie algebroids is a simultaneous generalization of tangent bundles and Lie algebras. In this subsection we briefly review the relevant notions. We refer to [51] for a detailed account.

Definition 5.1.1. Let M be a smooth manifold. A Lie algebroid $(A, \rho, [\cdot,\cdot])$ is given by a finite-dimensional vector bundle A, a vector bundle morphism $\rho : A \to TM$, called anchor and a ($\mathbb{R}$-bilinear) Lie bracket on the sections of A

$$[\cdot,\cdot] : \Gamma(A) \times \Gamma(A) \to \Gamma(A)$$

satisfying for all $f \in C^\infty(M)$, $s, s' \in \Gamma(A)$:

$$[s, fs'] = f[s, s'] + \rho(s)(f) \cdot s'.$$

It can be shown that the above condition implies that $\rho_* : \Gamma(A) \to \Gamma(TM) = \mathfrak{X}(M)$ is a Lie algebra homomorphism. Lie algebroids appear in many different settings:

- The tangent bundle TM with its usual bracket and $\rho = id$ is a Lie algebroid.
- Let $F \subset TM$ be an involutive subbundle, i.e. a foliation. Then F is a Lie algebroid with the restricted bracket and the inclusion $F \to TM$ as anchor.
- Let $\mathfrak{g}$ be a Lie algebra and $v : \mathfrak{g} \to \mathfrak{X}(M)$ an infinitesimal action (i.e. a Lie algebra homomorphism). Then $\mathfrak{g} \times M$ is a Lie algebroid with bracket induced by the Lie bracket on $\mathfrak{g}$ and anchor $\rho(\xi, p) = v(\xi)(p)$. In particular Lie algebras can be seen as Lie algebroids over a point.
- Let $\pi \in \Gamma(\Lambda^2 TM)$ be a Poisson bivector. Then the cotangent bundle of M carries a Lie algebroid structure induced by π. This is actually a particular instance of the Lie algebroid associated to a Dirac structure, which we will treat in the next subsection.

Lie algebroids can be alternatively defined as fiberwise linear Poisson structures on vector bundles or as differential graded manifolds of degree 1 (cf. e.g. [68]). In particular, there is a degree 1 differential (the Lichnerowicz differential, [48]) $d_A : \Gamma(\Lambda^\bullet A^*) \to \Gamma(\Lambda^{\bullet+1} A^*)$, where $\bullet$ denotes an appropriate integer index. This differential is defined by

$$\begin{aligned}(d_A\eta)(\xi_1, ..., \xi_{n+1}) = &\sum_i (-1)^{i+1} \rho(\xi_i)(\eta(\xi_1, ..., \hat{\xi_i}, .., \xi_{n+1})) \\ &+ \sum_{i<j} (-1)^{i+j} \eta([\xi_i, \xi_j], \xi_1, ..., \hat{\xi_i}, ..., \hat{\xi_j}, .., \xi_{n+1})\end{aligned}$$

The differential satisfies $d_A^2 = 0$ and induces a cohomology, which is called Lie algebroid cohomology and denoted by $H^\bullet(A)$. The anchor ρ induces a morphism from the usual de Rham cohomology to it: $H^\bullet_{dR}(M) \to H^\bullet(A)$.

A Lie algebroid always induces a singular foliation on M: The subspace $\rho(A) \subset TM$ is always involutive and – by construction – locally finitely generated, hence the integrability theorem (cf.

[34], reviewed in [44]) applies and M has a decomposition into immersed connected submanifolds $M = \bigsqcup_\alpha N_\alpha$ such that $TN_\alpha = \rho(A)|_{N_\alpha}$ for all N_α. Moreover, the bracket on A restricts to well-defined brackets on $A|_{N_\alpha}$, turning $A|_{N_\alpha} \to N_\alpha$ into Lie algebroids.

The submanifolds N_α are called leaves (of the foliation induced by the Lie algebroid) and a Lie algebroid is called transitive, if it has only one leaf, i.e. $\rho(A) = TM$ and M is connected.

5.1.2 The horizontal cohomology of Lie algebroid

Definition 5.1.2. Let $A \xrightarrow{\rho} TM$ be a Lie algebroid over the smooth manifold M. We define:

- The subspace of ρ-horizontal forms at $m \in M$ as:

$$(\Lambda^\bullet A_m^*)^{hor} := \{\alpha \in \Lambda^\bullet A_m^* \mid \iota_v \alpha = 0 \ \forall v \in \ker(\rho_m : A_m \to T_m M)\}$$

- The subspaces of ρ-horizontal forms:

$$\Gamma(\Lambda^\bullet A^*)^{hor} = \{\alpha \in \Gamma(\Lambda^\bullet A^*) \mid \alpha_m \text{ is horizontal for all } m\}$$

- the horizontal cohomology of A as the quotient

$$\mathcal{H}^\bullet_{hor}(A) = \frac{\ker(d_A : \Gamma(\Lambda^\bullet A^*)^{hor} \to \Gamma(\Lambda^{\bullet+1} A^*)^{hor})}{\mathrm{Image}(d_A : \Gamma(\Lambda^{\bullet-1} A^*)^{hor} \to \Gamma(\Lambda^\bullet A^*)^{hor})}$$

Remark 5.1.3. Of course, there are natural maps $H^\bullet_{dR}(M) \to \mathcal{H}^\bullet_{hor}(A)$ and $\mathcal{H}^\bullet_{hor}(A) \to H^\bullet(A)$. In general, these maps are neither injective nor surjective, as we will see in the sequel.

Example 5.1.4. When A is a transitive Lie algebroid (i.e. $\rho(A) = TM$), then $H^\bullet_{hor}(A)$ is isomorphic to the usual de Rham cohomology $H^\bullet_{dR}(M)$. More generally, if $\rho(A)$ is a regular foliation (i.e. if ρ has constant rank), then $H^\bullet_{hor}(A)$ recovers the longitudinal cohomology of the foliation induced by $\rho(A)$.

The above example actually extends to the following:

Lemma 5.1.5. *Let A be a Lie algebroid and $N \subset M$ a leaf of A and $\eta \in \Gamma((\Lambda^k A^*)^{hor})$ a ρ-horizontal form.*

1. *$\eta|_N$ is a ρ-horizontal k-form on the restricted Lie algebroid $A|_N \to N$, i.e. it induces a unique k-form $\eta_N \in \Omega^k(N)$.*
2. *η is completely determined by the collection $\{\eta_N \mid N \text{ leaf of } A\}$.*
3. *When η is horizontal, we have $(d_A \eta)_N = d\eta_N$.*
4. *Let $[\eta] = 0 \in \mathcal{H}^k_{hor}(A)$, then $[\eta_N] = 0 \in H^k_{dR}(N)$ for all leaves N of the algebroid A.*

Remark 5.1.6. In view of the above example and remark, let us stress that the usual intuition related to the "horizontal" as parallel to the base should be applied very carefully since it is sometimes misleading. This newly defined cohomology also should not be confused with basic or equivariant cohomology of algebroids (cf. [28, 78]).

5.1.3 Dirac structures

In this subsection, we briefly review the notion of Dirac structures. For details we refer to [17].

Let M be a manifold. The standard Courant algebroid (exact Courant algebroid with vanishing Ševera class) on M is given by $(\mathbb{T}M, \langle\cdot,\cdot\rangle, [\cdot,\cdot])$, where $\mathbb{T}M$ is $TM \oplus T^*M$ as a vector bundle, $\langle\cdot,\cdot\rangle : \mathbb{T}M \otimes \mathbb{T}M \to \mathbb{R}$ is[1] the standard symmetric pairing $\langle(v,\alpha),(w,\beta)\rangle = \alpha(w) + \beta(v)$ and $[\cdot,\cdot] : \Gamma(\mathbb{T}M) \otimes \Gamma(\mathbb{T}M) \to \Gamma(\mathbb{T}M)$ is the Courant bracket:

$$[(X,\alpha),(Y,\beta)] = ([X,Y], L_X\beta - L_Y\alpha - \frac{1}{2}d(\beta(X) - \alpha(Y))).$$

This bracket is skew-symmetric but does not satisfy the Jacobi identity. There is an alternative definition of bracket (the Dorfman bracket), which satisfies the Jacobi identity, but is not skew symmetric. We are now prepared to give the central definition of a Dirac structure:

Definition 5.1.7. A $dim(M)$-dimensional subbundle $D \subset \mathbb{T}M$ is called Dirac structure, if it is isotropic (i.e. $\langle D, D\rangle = 0$) and involutive (i.e. $[\Gamma(D), \Gamma(D)] \subset \Gamma(D)$).

Let us look at some examples:

- Let $\omega \in \Omega^2_{cl}(M)$ be a closed 2-form. Then its graph $\Gamma_\omega = \{(v, \iota_v\omega) \mid v \in TM\}$ is a Dirac structure. Any Dirac structure with bijective anchor $D \to TM$ (i.e. the restriction of the projection $\mathbb{T}M \to TM$ to D is bijective) can be described by the graph of a closed 2-form.
- Let $\pi \in \Gamma(\Lambda^2 TM)$ be a Poisson structure. Its graph $\Gamma_\pi = \{(\iota_\alpha\pi, \alpha) \mid \alpha \in T^*M\}$ is a Dirac structure. Any Dirac structure with bijective projection $D \to T^*M$ can be described as a Poisson bivector.
- Let $F \subset TM$ be an involutive (regular) distribution and $F^\circ \subset T^*M$ its annihilator. Then $D = F \oplus F^\circ$ is a Dirac structure.

Remark 5.1.8. The closedness of the 2-form ω is essential for Γ_ω to be involutive. However, for a non-closed 2-form, we can consider a twisted Courant algebroid $(\mathbb{T}M, \langle\cdot,\cdot\rangle, [\cdot,\cdot]_{d\omega})$ (with a twisting of the Courant bracket using $d\omega$) with respect to which Γ_ω is involutive, i.e. a (twisted) Dirac structure. In this chapter, we will only work with Dirac structures in the standard Courant algebroid.

Restricted to a Dirac structure D, the Courant bracket becomes a Lie bracket and turns D into a Lie algebroid. We call the (horizontal) Lie algebroid cohomology of D its (horizontal) Dirac cohomology. The Dirac structure also induces a canonical horizontal 2-cocycle that we will now describe.

5.1.4 The natural horizontal two-cocycle of a Dirac structure

Let $D \subset \mathbb{T}M$ be a Dirac structure. We define $\omega_D \in \Gamma(\Lambda^2 D^*)$ by

$$\omega_D((v,\alpha),(w,\beta)) = \alpha(w) - \beta(v).$$

As D is isotropic, we have $\omega_D((v,\alpha),(w,\beta)) = 2\alpha(w) = -2\beta(v)$, i.e. ω_D is horizontal at each point. A computation based on the involutivity of D ([8]), shows that ω_D is closed in Dirac cohomology, i.e.

[1] $\otimes$ stands for the tensor product.

$d_D\omega_D = 0$, and hence ω_D is horizontal.[2] It thus yields a natural class in $\mathcal{H}^2_{hor}(D)$. Hence, in view of Lemma 5.1.5 we have:

Lemma 5.1.9. *Let $D \subset \mathbb{T}M$ be a Dirac structure.*

1. *There is a naturally induced horizontal cocycle $\omega_D \in \Gamma(\Lambda^2 D^*)^{hor}$ associated to any Dirac structure D.*
2. *If $[\omega_D] = 0 \in \mathcal{H}^2_{hor}(D)$, then for any leaf N of D, $[(\omega_D)_N] = 0 \in H^2_{dR}(N)$.*

Remark 5.1.10. The second statement above heavily relies on the fact that we work with the horizontal cohomology: Even when a primitive of ω_D in $\Gamma(\Lambda^\bullet D^*)$ exists, it has no reason to be horizontal (i.e. to restrict to leaves) in general.

Remark 5.1.11. The construction of the above 2-form works out, even when D is an *almost-Dirac structure*, i.e. an isotropic $dim(M)$-dimensional subbundle of $\mathbb{T}M$ (which might not be involutive). However, in this case D can fail to be a Lie algebroid and hence there is no associated Lie algebroid cohomology to lie in.

5.1.5 Examples

Let us interpret the class $[(\omega_D)]$ in the most important cases.

Example 5.1.12. $D = \Gamma_\omega \subset \mathbb{T}M$ is the graph of a (pre-)symplectic structure ω. Then the Lie algebroid structure on D is isomorphic to the Lie algebroid TM. Hence, the horizontal cohomology is canonically isomorphic to the de Rham cohomology ($\mathcal{H}^\bullet_{hor}(D) \cong H^\bullet(D) = H^\bullet_{dR}(M)$). The form ω_D corresponds to ω under this isomorphism.

Example 5.1.13. Let $D = F \times F^\circ \subset \mathbb{T}M$, where $F \subset TM$ is a regular foliation. The Lie algebroid structure on D is the induced bracket on F (the usual Lie bracket of vector fields) and the zero bracket on F°. Then $H^\bullet(D) \cong H^\bullet(F) \times \Lambda^\bullet(F^\circ)^*$ and $\mathcal{H}^\bullet_{hor}(D) \cong H^\bullet(F)$. The form ω_D is zero.

Remark 5.1.14. If $F \subset TM$ is not involutive, then $D = F \times F^\circ$ is still an almost-Dirac structure (cf. Remark 5.1.11). Even though there is no cohomology, the associated 2-form ω_D is still zero.

Example 5.1.15. Let $D \subset \mathbb{T}M$ be the graph of a Poisson structure π. Then the Lie algebroid D is isomorphic to T^*M and $H^\bullet(D) \cong H^\bullet_\pi(M)$ is known as the Poisson cohomology (see for example [22]). The class of ω_D in $H^\bullet(D)$ corresponds to the class of π in $H^2_\pi(M)$. The class of ω in the finer cohomology $\mathcal{H}^\bullet_{bas}(D)$ is zero if and only if $\pi \in \mathfrak{X}^2(M)$ admits a primitive $E \in \mathfrak{X}(M)$ (a vector field E satisfying $L_E\pi = \pi$), which is tangent to the Poisson structure, i.e. is a section of $\rho(D) \subset TM$.

For instance for $M = \mathbb{R}^2$, the Poisson structure $\pi = x^2\partial_x \wedge \partial_y$ admits such a primitive $E = x\partial_x$.

Also, on each leaf N of D, ω_D restricts to a symplectic form ([8]). And hence there are no exact symplectic structures on compact manifolds, this leads to the following obstruction to the existence of horizontal primitives of ω_D: for a Poisson structure with vanishing cohomology class, the only compact leaves of its symplectic foliation are points.

[2] Note that from now on we write horizontal as a shorthand for ρ-horizontal, since the anchor map is no longer explicitly used.

Example 5.1.16. Here is a classical type of Poisson structures: let $\mathfrak{g}$ be a Lie algebra. Its dual $M = \mathfrak{g}^*$ carries a natural Poisson structure, whose leaves are the coadjoint orbits of $G \curvearrowright \mathfrak{g}^*$ (cf. e.g. [43]).

In this case $[\pi] \in H^2_\pi(M) = H^2(D)$ is always zero: There exists a (linear) vector field E, such that $[\pi, E] = \pi$. However, E can rarely be chosen to be tangent to the coadjoint orbits. For instance, when $\mathfrak{g}$ is compact and semi-simple, this can never occur.

5.2 A variational approach to exact Dirac structures

5.2.1 Dirac paths

Theorem 5.2.1. *Let $D \subset \mathbb{T}M$ be a Dirac structure over M, $H \in C^\infty(M)$ be a Hamiltonian function and γ a path on M.*

Assume that the horizontal 2-class $[\omega_D]$ vanishes, and let $\theta \in \Gamma(D^*)^{hor}$ be such that $d_D\theta = \omega_D$, then the following statements are equivalent:

(i) The path γ is a Hamiltonian curve, i.e. $(\dot\gamma(t), dH_{\gamma(t)}) \in D$ for all t.

(ii) All Dirac paths $\zeta : I \to D$ over γ (i.e. $\rho(\zeta) = \dot\gamma$) are critical points among the Dirac paths with the same end points of the following functional:

$$\zeta \mapsto \int_I \big(\theta_{\gamma(t)}(\zeta(t)) + H(\gamma(t))\big)\, dt \tag{5.1}$$

(iii) There exists a Dirac path $\zeta : I \to D$ over γ and the latter is the critical point, among Dirac paths with the same end points, of the functional (5.1).

Proof. As $\theta(\zeta)$ does not depend on the choice of a Dirac path ζ over γ, the equivalence of (ii) and (iii) is obvious.

For the equivalence between (i) and (iii), let us first note that we can restrict the functional (5.1) to a fixed leaf N containing γ. On N, $\omega_{\mathcal{D}}$ corresponds to a pre-symplectic form ω_N and θ yields a potential of ω_N, i.e. a 1-form $\theta_N \in \Omega^1(N)$ such that $d\theta_N = \omega_N$. Thus, it suffices to prove the assertion of the theorem for an exact pre-symplectic form $\omega_N = d\theta_N$. That is to say, we want to prove, that the image of $\dot\gamma$ by the musical isomorphism $\omega_N^\flat$ equals $\mathrm{d}H$ along γ: $\omega_N^\flat(\dot\gamma) = \mathrm{d}_\gamma H$ if and only if $\gamma : I \to N$ is a critical point of

$$\int_I \big(\theta_N|_{\gamma(t)}(\dot\gamma(t)) + H(\gamma(t))\big)dt$$

among curves with fixed endpoints. For symplectic manifolds this is a classical result [2], we provide a proof (that follows the same lines) for the sake of completeness.

Take a small variation

$$v : \begin{array}{ccc} I \times (-\epsilon, \epsilon) & \to & N \\ (t, s) & \mapsto & v(t, s) \end{array}$$

of γ with fixed endpoints and set $Y(t) = \frac{\partial}{\partial s}\big|_{s=0} v \in T_{\gamma(t)}N$. We call $\gamma^* L_Y \theta_N$ the smooth $\mathbb{R}$-valued function on I defined by

$$\gamma^* L_Y \theta_N(t) = \frac{\partial}{\partial t}\theta_N|_{\gamma(t)}(Y(t)) + d\theta_N(Y(t), \dot\gamma(t)).$$

(If Y happens to be the restriction to γ of a vector field Y on N, $\gamma^* L_Y \theta_N(t)dt \in \Omega^1(I)$ is the pull-back through $\gamma : I \to N$ of $L_Y\theta_N$, hence the notation.)

$$\begin{aligned}
&\frac{\partial}{\partial s}\Big|_0 \int_{t\in I} \left(\theta_N|_{v_s(t)}\left(\frac{\partial v_s}{\partial t}(t)\right) + H(v_s(t))\right) dt \\
&= \int_{t\in I} \frac{\partial}{\partial s}\Big|_0 \left(\theta_N|_{v_s(t)}\left(\frac{\partial v_s}{\partial t}(t)\right) + H(v_s(t))\right) dt \\
&= \int_{t\in I} \left(\gamma^* L_Y\theta_N(t) + dH|_{\gamma(t)}(Y(t))\right) dt \\
&= \int_{t\in I} \left(d\theta_N(Y(t),\dot\gamma(t)) + dH|_{\gamma(t)}(Y(t))\right) dt
\end{aligned}$$

In the two last equalities, we used integration by parts and the fact that $Y(0) = 0$ and $Y(1) = 0$ since the endpoints of v are fixed, so that $\int_I \frac{\partial}{\partial t}\theta_N|_{\gamma(t)}(Y(t))dt = 0$. Since $Y(t)$ is arbitrary except at end points, this proves the result. □

Remark 5.2.2. In the above proof, we actually do not require the equality $d\theta = \omega$ and the horizontality of θ globally. We only need both properties along the leaf N one considers.

Example 5.2.3 (Hamiltonian classical mechanics)**.** We recover a classical framework ([35]) by the following: let $M = T^*Q$, $H \in \mathcal{C}^\infty(T^*Q)$ and $\gamma(t) = (q(t), p(t))$ be a path on T^*Q, where (q, p) are position-momenta coordinates on the phase space T^*Q. Then, γ is a Hamiltonian trajectory of H :

$$\begin{cases} \dot q &= -\frac{\partial H}{\partial p} \\ \dot p &= \frac{\partial H}{\partial q} \end{cases}$$

if and only if γ is a critical point of the functional

$$\gamma \mapsto \int_I \left(\theta_{\gamma(t)}(\dot\gamma(t)) + H(\gamma(t))\right) dt,$$

where $\theta = p\mathrm{d}q$ is the Liouville 1-form.

The above proof enables us to treat a much wider class of Dirac structures than in section 5.1.5, especially singular ones.

Example 5.2.4 (Restriction to a leaf)**.** Consider $\mathbb{R}^4$ with the Poisson structure

$$\pi = (x^2 + y^2)\partial_x \wedge \partial_y + \partial_z \wedge \partial_w.$$

Along the singular leaf $L = \{x = y = 0\}$ the vector field $w\partial_w$ is horizontal and a primitive for π on that leaf, hence the above remark applies and we obtain a variational characterization of paths.

5.2.2 Tulczyjew isomorphisms and Legendre transformation

Tulczyjew isomorphisms

For self-containedness of this chapter, we recall here the isomorphisms established by W. Tulczyjew ([66, 67]) between double (co)tangent bundles (at least one "co" should be present).

We first present the canonical flip, which is a canonical involution:

$$\sigma\colon T(TQ) \simeq T(TQ).$$

It can be seen as a sort of Schwarz Lemma: for every smooth map $\Sigma(s,t) := \mathbb{R}^2 \to Q$ (defined in a neighborhood of $(0,0)$):

1. $t \mapsto \frac{\partial\Sigma(0,t)}{\partial s}$ is a path in TQ starting from $\frac{\partial\Sigma}{\partial s}(0,0)$. Its first jet at 0 belongs to $T_{\frac{\partial\Sigma}{\partial s}(0,0)}(TQ)$.
2. $s \mapsto \frac{\partial\Sigma(s,0)}{\partial t}$ is a path in TQ starting from $\frac{\partial\Sigma}{\partial t}(0,0)$. Its first jet at 0 belongs to $T_{\frac{\partial\Sigma}{\partial t}(0,0)}(TQ)$.

By definition, the canonical flip is an unique map that exchanges both elements in $T(TQ)$:

$$\sigma\left(\frac{\partial}{\partial t}\frac{\partial\Sigma(s,t)}{\partial s}\bigg|_{s=t=0}\right) = \frac{\partial}{\partial s}\frac{\partial\Sigma(s,t)}{\partial t}\Sigma(s,t)\bigg|_{s=t=0}$$

A canonical isomorphism:

$$\kappa\colon TT^*Q \to T^*TQ.$$

is then obtained through the following construction: TTQ is what is called a double vector bundle, for it has two compatible vector bundle structures over TQ. Consider the respective duality pairings

$$<\cdot,\cdot>_1\colon T(T^*Q)\otimes T(TQ) \longrightarrow \mathbb{R}$$

and

$$<\cdot,\cdot>_2\colon T^*(TQ)\otimes T(TQ) \longrightarrow \mathbb{R}.$$

Then the mapping κ is implicitly canonically defined by imposing

$$<\kappa(a), b>_2 = <a, \sigma(b)>_1$$

for all $a \in T(T^*Q)$ and $b \in T(TQ)$ which are in the same fiber of their canonical projections on TQ.

More Tulczyjew isomorphisms of vector bundles are obtained by post- or pre-composing $\Omega^\flat\colon TT^*Q \to T^*T^*Q$ or its inverse, where Ω is the canonical symplectic form on T^*Q. We will be mostly interested in the isomorphism

$$\beta \equiv \omega^\flat \circ \kappa^{-1}\colon T^*TQ \to T^*T^*Q \tag{5.2}$$

which is a particular case of the canonical isomorphism also called Tulczyjew isomorphism $T^*E \simeq T^*E^*$ for any vector bundle E([52]) that we describe now.

Relation inbetween Tulczyjew isomorphisms and Legendre transformation

Throughout this paragraph, U is a fiberwise convex open subset of a vector bundle E over Q, equipped with a smooth function $L\colon U \subset E \to \mathbb{R}$ called *Lagrangian*.

Recall that if a smooth function f on an open convex subset $U \subset V$ of a vector space is strictly convex, then its differential, defined for all $v \in U$ by:

$$\begin{aligned}\mathbb{F}f\colon U &\to V^*\\ v &\mapsto \left(e \mapsto \frac{d}{dt}\bigg|_{t=0} f(v+te)\right)\end{aligned}$$

is a diffeomorphism from U onto its image U'. Applying this result at every fiber of E, we obtain that if the restriction of L to any fiber is strictly convex, then $\mathbb{F}L : U \subset E \hookrightarrow E^*$ is a diffeomorphism from U to its image $U' \subset E^*$.

In this context, we define the Legendre transform $H \in C^\infty(U')$ of L to be the unique function satisfying $H(\alpha) + L(v) = \langle \alpha, v \rangle$ for all $\alpha \in E^*$ with $\alpha = \mathbb{F}L(v)$.

Proposition 5.2.5. *The Legendre transform and the Tulczyjew isomorphism are related by the equality*

$$\beta(d_e L) = d_{\mathbb{F}L(e)} H$$

for every $e \in U$.

When L is not strictly convex on a fiberwise cnvex open subset, the Legendre transform does not need to exist. However the set $\{\beta(d_e L) \mid e \in U\}$ is always a Lagrangian submanifold of T^*E^*. It appears throughout this chapter as the image of $\mathcal{D}L$.

5.2.3 Generalized implicit Lagrangian systems

Let $L\colon TQ \to \mathbb{R}$ a (possibly degenerate) Lagrangian.

Remark 5.2.6. Note that in this section and in the next one the base manifold will be systematically Q instead of M used before – this is to stress the fact that in the Lagrangian picture it is necessary to lift the construction to double vector bundles, and thus the relevant Dirac structures will be over Q or T^*Q depending on the context. The general facts about Dirac structures will still be formulated with the base manifold denoted by M.

Definition 5.2.7. We call Tulczyjew's differential the map $u \mapsto \mathcal{D}_u L := \beta(d_u L)$, where $\beta : T^*TQ \to T^*T^*Q$ is the Tulczyjew isomorphism 5.2. Its image is a submanifold of T^*T^*Q.

Definition 5.2.8. We also define a map from TQ to T^*Q by $\mathbb{F}L(v)$ for every $v \in T_qQ$ by

$$\frac{\partial}{\partial t}\Big|_{t=0} L(v + tw) = \langle \mathbb{F}L(v), w \rangle$$

a) We denote by $\mathfrak{Leg} = \mathbb{F}L(TQ) \subset T^*Q$ the image of $\mathbb{F}L$.

b) We call partial vector fields on $\mathfrak{Leg}$ sections[3] of $\Gamma(T(T^*Q))|_{\mathfrak{Leg}}$.

c) An integral curve of a partial vector field X on $\mathfrak{Leg}$ is a path $t \mapsto u_t \in TQ$ such that

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbb{F}L(u_t) = X_{\mathbb{F}L(u_t)}.$$

d) An implicit Lagrangian system for an almost Dirac structure $\mathbb{D} \subset \mathbb{T}T^*Q$ is a pair (X, L), with X a partially defined vector field on $\mathfrak{Leg}$, such that $(X(\mathbb{F}L(u)), \mathcal{D}_u L) \in \mathbb{D}$ for all u in TQ.

Remark 5.2.9. We do not assume partial vector fields on $\mathfrak{Leg}$ to be tangent to $\mathfrak{Leg}$ in any sense. Of course, if they are not tangent, they may have little integral curves.

[3]For E a vector bundle over a manifold X and $Y \subset X$ an arbitrary subset (not necessarily a manifold), we denote by $\Gamma(E)|_Y$ restrictions to Y of smooth sections of E in a neighborhood of Y in X.

Remark 5.2.10. Particular cases include:

- Usual Hamiltonian dynamics. When $\mathbb{F}L$ is a diffeomorphism and $\mathbb{D}$ is the graph of the canonical symplectic form on T^*Q, implicit Lagrangian systems are pairs (X_H, L), where X_H is the Hamiltonian vector field of H, the Hamiltonian function associated to L via the Legendre transform.
- Constraint dynamics, which actually motivated the construction, we give some details below: Example 5.2.17.

5.2.4 Implicit Lagrangian systems with magnetic terms

Definition 5.2.11 ([8])**.** Let $D \subset \mathbb{T}M$ be a subbundle.

1. For all $\phi\colon M' \to M$, we denote by $\phi^!D$ the set

$$\phi^!D_{m'} := \left\{(X, \phi^*\beta) \text{ with } X \in T_{m'}M', \beta \in T^*_{\phi(m')}M \text{ s.t.}(\phi_*(X), \beta) \in D_{\phi(m')}\right\}$$

   When D is an (almost-)Dirac structure we call $\phi^!D$ the pullback of D.

2. Let ω be a 2-form $\omega \in \Omega^2(M)$, we denote by $e^\omega D$ the set

$$e^\omega D = \{(v, \beta + \iota_v\omega) \mid (v, \beta) \in D\}$$

   and call it the gauge transform of D.

Lemma 5.2.12 (cf. e.g. [8])**.** *Let $D \subset \mathbb{T}M$ be a Dirac structure and M' be a manifold.*

1. *For any smooth map $\phi\colon M' \to M$, $\phi^!D$ is a Dirac structure on M'.*
2. *For any closed 2-form $\omega \in \Omega^2(M)$, $e^\omega D$ is a Dirac structure on M.*

Given $D \subset \mathbb{T}Q$ a Dirac structure on Q, this lemma allows to consider *(i)* its pull back $\pi^!D$ on T^*Q through the canonical base map $\pi\colon T^*Q \to Q$, then *(ii)* consider the gauge transformation $e^\Omega\pi^!D$ of this pull-back with respect to the canonical symplectic 2-form Ω.

Definition 5.2.13. Let $D \subset \mathbb{T}Q$ be a Dirac structure on Q. We call constrained magnetic Lagrangian system an implicit Lagrangian system for the Dirac structure $\mathbb{D} = e^\Omega\pi^!D \subset \mathbb{T}T^*Q$ as above.

Theorem 5.2.14. *Let $D \subset \mathbb{T}Q$ be a Dirac structure and $L : TQ \to \mathbb{R}$ a Lagrangian. Assume that the 2-form $\omega_D \in \Gamma(\Lambda^2 D^*)^{hor}$ admits a horizontal primitive $\theta \in \Gamma(D^*)^{hor}$. Then for $q : I \to Q$ the following are equivalent:*

a) There exists a Dirac path $\zeta : I \to D$ such that $\rho(\zeta) = \dot{q}$ which is the critical point among Dirac paths with the same end points of

$$\int_I (L(\rho(\zeta(t))) + \theta(\zeta(t)))dt. \tag{5.3}$$

b) For all $t \in I$, the following condition holds.

$$\left(\frac{\partial}{\partial t}\mathbb{F}L(\dot{q}(t)), \mathcal{D}_{\dot{q}(t)}L\right) \in \mathbb{D} = e^\Omega\pi^!D. \tag{5.4}$$

Proof. We claim that it suffices to check the equivalence on a small open set in Q. The second assertion is clearly local in nature and a path is a critical point for the functional (5.3) if and only if for any $t \in I$ there is a subinterval $t \in I_t \subset I$ on which it is critical[4].

It suffices therefore to establish the equivalence on an open subset U of Q, on which the Dirac structure takes the following normal form ([7]):

- $U = S \times N$, where $S \subset \mathbb{R}^a, N \subset \mathbb{R}^b$ with $q(0)$ lying in $S \times \{0\}$.
- $D|_U = e^{\eta}((TS \oplus \{0\}) \times \Gamma^{\Pi})$, where $\eta \in \Omega^2_{cl}(U)$ and $\Pi \in \mathfrak{X}^2(N)$ is a Poisson bivector field vanishing at 0 and Γ^{Π} is the corresponding Dirac structure on N.

As $S \times \{0\}$ is a leaf of D, $q(t) \in S \times \{0\}$ for all t. By our assumptions on D

$$\int_I (L(\rho(\zeta(t))) + \theta(\zeta(t)))dt = \int_I (L(\dot{q}) + \theta^S(\dot{q}))dt,$$

where $\theta^S \in \Omega^1(S)$ is the one-form on S induced by θ and hence satisfies $d\theta = i_S^* \eta$ where $i_S : S \to U, i_S(s) = (s, 0)$.

We will denote by L^S the restriction of L to TS and write $q = (q^S, 0)$. With these conventions, the above functional reads:

$$\int_I (L^S(\dot{q}^S) + \theta^S(\dot{q}^S))dt.$$

The classical Euler-Lagrange theorem ([58]) with magnetic term implies that being a critical point of this functional is equivalent to

$$\left(\frac{\partial}{\partial t}\mathbb{F}L^S(\dot{q}^S(t)), \mathcal{D}_{\dot{q}^S(t)}L^S\right) \in e^{\Omega}\pi^! e^{\eta^S}(TS \oplus \{0\}). \tag{5.5}$$

Via the isomorphism $\mathbb{T}T^*U = \mathbb{T}T^*S \times \mathbb{T}T^*N$, the assertion (5.4) decomposes as two conditions, the first one (on S) being (5.5). The second condition (on N) is always satisfied, as one can verify by a straightforward computation in local coordinates which relies on the fact that q is constant on N.

□

Corollary 5.2.15. *Let Q, L, D be as in Theorem 5.2.14 and (X, L) an implicit Lagrangian system. Then any integral curve γ of X is the base path of a critical point of* (5.3).

Example 5.2.16 (Classical symplectic magnetic terms)**.** Theorem 5.2.14 allows to recover variational formulation of the dynamics of a particle in a magnetic field, see section 6.7 of [54] for their Hamilton equations. We give a geometric explanation of this particular case using the notion of implicit Lagrangian system.

Let Q be any manifold, $\omega \in \Omega^2_{cl}(Q)$ and $D = \Gamma_\omega \subset \mathbb{T}Q$. Let $L : TQ \to \mathbb{R}$ be a Lagrangian. In this case $e^{\Omega}\pi^! D = \Gamma_{\Omega + \pi^*\omega} \subset \mathbb{T}T^*Q$.

As $\mathcal{H}^{\bullet}_{basic}(D) = H^{\bullet}_{dR}(M)$, (cf. Example 5.1.12), the 2-form on D admits a basic potential if and only if ω is de-Rham exact, i.e. $\omega = d\theta$, $\theta \in \Omega^1(Q)$.

[4] That can be seen as follows: for two subinterval J_1 and J_2 of I, $\int_{J_1 \cup J_2}(L(\rho(\zeta(t))) + \theta(\zeta(t)))dt = \int_{J_1}(L(\rho(\zeta(t))) + \theta(\zeta(t)))dt + \int_{J_2}(L(\rho(\zeta(t))) + \theta(\zeta(t)))dt - \int_{J_1 \cap J_2}(L(\rho(\zeta(t))) + \theta(\zeta(t)))dt$

Let us assume that the Legendre transform $\mathbb{F}L : TQ \to T^*Q$ is bijective, and denote the Legendre transform of the Lagrangian by H, i.e.

$$H(p) = \langle p, (\mathbb{F}L)^{-1}p\rangle - L \circ (\mathbb{F}L)^{-1}(p)$$

In this case $\mathcal{D}L$ is simply dH. Theorem 5.2.14 yields that the critical points of $L(q,\dot{q}) + \theta(\dot{q})$ correspond under the Legendre transform to integral curves of the Hamiltonian flow of H for the symplectic structure $\Omega + \pi^*\omega$. Corollary 5.2.15 states that (X, dH) is an implicit Lagrangian system with respect to $e^{\Omega}\pi^!D$ if and only if the vector field X is the Hamiltonian vector field of H with respect to $\Omega + \pi^*\omega$.

Example 5.2.17 (Holonomic constraints as a regular foliation)**.** Let $F \subset TQ$ be a regular foliation. As discussed in Example 5.1.13, the Dirac structure $D = F \oplus F^\circ$ always admits a horizontal primitive, as the 2-form in $\Lambda^2 D^*$ is zero (there is no magnetic term). Then $\pi^!D$ is the Dirac structure associated to the pullback foliation $\pi^{-1}(F)$ and

$$e^{\Omega}\pi^!D = \{(w,\alpha) \in TT^*Q \oplus T^*T^*Q \mid \pi_*(w) \in F, \alpha - \Omega^\flat w \in \pi^{-1}(F)^\circ\}$$

Let $L : TQ \to \mathbb{R}$ be a Lagrangian. Then Theorem 5.2.14 and Corollary 5.2.15 yield that the integral curves of any implicit Lagrangian system $(X, \mathcal{D}L)$ for $e^{\Omega}\pi^!D$ are critical points of L among curves that are tangent to F. The condition (5.4) translates directly to the Euler-Lagrange equations for a system subject to holonomic constraints, which are classically spelled-out using the Lagrange multipliers [42].

Remark 5.2.18. Holonomic and non-holonomic constraints. Note that the result above concerns the so-called holonomic constraints, i.e. the conditions defining the constraints do not depend essentially on the velocities of the system. Geometrically this means that the foliation F comes from an integrable constraint distribution $\Delta \subset TQ$. Simple mechanical examples and counterexamples can be constructed by "rolling without slipping" problems: They are often formulated as an orthogonality condition on the velocity at the contact point – the condition is integrable for the rolling disk but not for a rolling ball. Under some extra assumptions the non-holonomic constraints can still be treated in the variational approach ([76]), though with no geometric interpretation. In this setting our result is more subtle, since as mentioned above, remarks 5.1.11 and 5.1.14, the non-integrable almost Dirac structures are very different from the cohomological perspective. Formally, we cannot speak of an obstruction class, since the "differential" does not square to zero. However when some primitive can be defined, parts of theorems 5.2.1 and 5.2.14 are still valid.

5.2.5 Applications to numerics

One of the motivations for the above construction is its potential application to design appropriate structure preserving numerical methods – so called geometric integrators.

Historically, the first example of those are the symplectic numerical methods, they are known since several decades, and are now state of the art for Hamiltonian systems ([75]). The key idea is that in the continuous setting the Hamiltonian flow not only preserves the level sets of the Hamiltonian function, but also leaves invariant the symplectic form. It is thus natural to mimic this property for the discrete flow, i.e. computing the trajectory numerically one wants to take the symplectic form into

account. And since it is actually the same symplectic form that defines the dynamics of the system, one can reverse the argument: a flow preserving the symplectic form will "respect" the level sets of the Hamiltonian defining it.

The Lagrangian counterpart of this picture is related to so-called variational integrators ([55]), the idea is rather natural as well. Instead of considering a continuous Lagrangian and searching for its extrema along all the paths with fixed endpoints:

$$\inf \mathcal{L} \equiv \inf \int_0^T L(q(t), \dot{q}(t))\mathrm{d}t \tag{5.6}$$

one defines the discrete version L_d of the integrant L as follows:

$$L_d(q_{n+1}, q_n, v_n) := \Delta t_n L(q_n, v_n).$$

Here $q_n \equiv q(t_n)$, v_n is some approximation of $\dot{q}(t_n)$ depending on q_n and q_{n+1}; and Δt_n are the time intervals between q_n and q_{n+1}, not necessarily all equal. One then defines the discrete analogue of variational principle (DVP), i.e. studies the trajectories $(q_0, q_1 \ldots, q_{n-1}, q_n)$ extremizing

$$\mathcal{L}_d = \sum_{n=0}^{N} L_d,$$

subject to $q_0 = q(0)$ and $q_N = q(T)$. For conservative mechanical systems one can recover usual symplectic methods with this variational approach, and it is actually more universal, since the timestep is allowed to vary as well.

A similar strategy can be applied whenever the variational principle can be formulated. For example, in [55] the case of systems with constraints is explored, which motivated some parts of this chapter; later on similar ideas were explored for continuous media problems (see e.g. [11]) Hence, the results of Sections 5.2.3 and 5.2.4 on the dynamics on Dirac structures fit to the picture perfectly: they basically say that as soon the cohomological obstruction is absent, one can formulate the Dirac dynamics with a variational approach. In Equation (5.6) one merely replaces the path $q(t)$ in the configuration manifold by a Dirac path $\zeta(t)$. In the continuous setting the Dirac paths preserve the Dirac structure by definition, the variational formulation permits to guarantee this property for the trajectory computed numerically.

There is however an important detail to mention: the folkloric perception of geometric integrators as "preservation of the geometric structure guarantees preservation of physical properties" is slightly simplified. For instance in the symplectic case, it is not the original Hamiltonian that is preserved, but its discrete version, for which one can estimate the difference [59]. The phenomenon is even more subtle in the variational case. In fact, saying that satisfying the discrete variational principle (DVP) results in preserving some quantities of the system is no longer that straightforward. In the generic case the DVP will only give the relations between different variables of the system, but they will still depend on the choice of discretization or approximation of some of them. It may (and often does) also happen that the choice of the discretization to preserve the structure exactly is technically very difficult or even a priori impossible. This means that the correct statements will concern rather preservation of geometric structures up to some order of discretization step.

A typical example of this situation is provided by the so-called constraint algorithms: for dynamical systems, the methods to take into account the constraints expressed as algebraic conditions on dynamical variables. When it is impossible to explicitly resolve the constraints, i.e. introduce the

dynamical variables satisfying them automatically, there are essentially two approaches: introduce the penalization terms with Lagrange multipliers and discretize them appropriately or "project" the solution to the level set of the algebraic conditions at each time step. However, to the best of our knowledge, there are very few proven theorems on how the discrete version of the system satisfies the constraints. We have tried to fill some gaps in empirical observations that one sees in literature. For example ([62]) the Dirac structure based algorithm ([76]) in the absence of constraints is naturally symplectic. And some partial results on how to construct *pseudo-geometric* integrators preserving the conditions *up to some order* are given in [50].

With the approach of the current chapter we now understand why the naive attempts to increase the order of the constraint-based methods (like e.g. [45]) do not produce the desired results: roughly speaking the obtained integrators fail to be geometric/variational in the proper sense of the word. A way out would be to formulate the DVP for the calculus of variations in a more general case ([58]), and then apply it to the context of Theorems 5.2.1 and 5.2.14.

CHAPTER 6

Conclusion and perspectives

6.1 Perspectives on the variational approach to Hamiltonian Dirac dynamics

We have defined in chapter 5 the basic Dirac cohomology, which permits to describe an explicit and verifiable condition for variational formulation of dynamics on Dirac structures.

As mentioned in the last part of the chapter, on top of purely mathematical interest, this construction should be useful to design more reliable tools for numerical integration of the flow of dynamical systems on Dirac structures. Those in turn naturally appear when studying constraint, interacting or dissipative mechanical systems, which are not in the range of classical Hamiltonian formalism. We expect the results of this chapter to provide a unified approach to those and in particular an extension of the observations from Section 5.2.5 to arbitrary Dirac structures with vanishing horizontal cocycle.

Let us also mention that, since Poisson manifolds provide an example of Dirac structures, this approach is useful to construct some Poisson integrators. In the context of this chapter there is no conceptual difference between the Dirac structures coming from constraint distributions or from symplectic foliations of Poisson manifolds. The constructed discretizations should thus preserve the symplectic leaves. This is somewhat complementary to the strategy of chapter 4, where the main tool is rather Hamiltonian dynamics and symplectic groupoids.

We suppose that these technical questions deserve a separate study ([33]) of the description of the discrete variational principal for the general case and the related discussion of the implementation issues. Some work on Dirac computational dynamics has been started (see [50]) while a study on applications and consequences in numerical analysis of chapter 5 still needs to be done.

We also remark that cohomological assumptions of theorems 5.2.1 and 5.2.14 are sufficient but not necessary. For instance, the construction applies to quasi Dirac structures, i.e. non-involutive ones. In addition, the integration of the cocycle $[\omega_D]$ can be considered while the Dirac structure is restricted to a leaf. We hope those last remarks to enlarge the class of potential applications.

6.2 Hamiltonian Poisson integrators : analysis for discrete trajectories and Zeitlin's model

This sections provides a conclusion and some future directions of research about Poisson integrators.

Some computations on Lagrangian bi-sections of a local model of the local symplectic groupoid of a Poisson structure π lead us to the Hamilton-Jacobi equation. Given a bi-realisation $\mathcal{W}$ and a Hamiltonian H, it gave in turn the construction, for any order k and any time-step ϵ, of a Hamiltonian Poisson integrator φ_ϵ^k of H. This construction provides two properties to φ_ϵ^k :

- it is a Poisson automorphism,
- x and $\varphi_\epsilon^k(x)$ are on the same leaf of the Poisson structure.

We also observed numerically a good stability around a singularity of the considered system.

Using Magnus formula, we think the existence of a time-dependent Hamiltonian recovering φ_ϵ^k might be deeply related to the behaviour of Hamiltonian Poisson integrators for long run simulations and we plan to work on consequences of this existence property.

This work is presented for finite dimensional Poisson structures, while an interesting class of problems in computational dynamics lie in the framework of infinite dimensional Poisson geometry (see [1] for lectures on Poisson geometry in fluid mechanics). We suggest a relation between both by the example of Zeitlin's model ([77]) for incompressible fluid.

Hamiltonian Poisson integrators might be used there ([12]) and provide interesting geometric features. The question of the relation inbetween the existence of a time-dependent Hamiltonian recovering a Hamiltonian Poisson integrator and its behaviour for long run simulations is also relevant in that framework. Furthermore, a better theoretical understanding of Zeitlin's model may lead to its extension at other Poisson partial differential equations and open a new direction towards geometric integrators for those PDEs.

Appendices

.1 Local symplectic groupoids

This appendice aims at summarizing the theory and prove the theorems we need about local symplectic groupoids for the construction of Hamiltonian Poisson integrators. It is mainly based on [69, 16, 61, 22]. A better presentation will be given soon, as well as a better statement and a proof of theorem .1.20.

.1.1 Local Lie groupoids

Definition .1.1 (Local Lie groupoid, [69])**.** A local Lie groupoid is the following data:

- a manifold $\mathcal{G}$ called the *space of arrows*,
- a manifold M called the *base space*,
- two surjective submersions α and β from $\mathcal{G}$ to M, respectively called the *source* and *target*,
- a neighborhood $\mathcal{V}$ of $\mathcal{G} \times M \bigcup M \times \mathcal{G}$ in the fiber product $\mathcal{G} \,{}_{\alpha}\!\times_{\beta}\, \mathcal{G}$ and a smooth map $m\colon \mathcal{V} \to \mathcal{G}\colon (a,b) \mapsto a \cdot b$ called the *local product*,
- a map $\mathrm{inv}\colon \mathcal{V} \circlearrowleft\colon a \mapsto a^{-1}$ called the *inverse*.

This data is assumed to verify the following properties: for every $(a,b,c) \in \mathcal{G}^3$ such that (a,b), (b,c), $(a \cdot b, c)$ and $(a, b \cdot c)$ are in $\mathcal{V}$,

- $(a.b).c = a.(b.c)$, i. e. the local product is associative,
- $\alpha(a \cdot b) = \alpha(a)$ and $\beta(a \cdot b) = \beta(b)$,
- $a \cdot i(\beta(a)) = i(\alpha(a)) \cdot a = a$,
- $a \cdot a^{-1} = i(\alpha(a))$ and $a^{-1} \cdot a = i(\beta(a))$.

This local Lie groupoid will be denoted by its space of arrows $\mathcal{G}$.

Remark .1.2. It can be shown, see chapter III of [51], that :

1. the inverse is a diffeomorphism,
2. the identity section is an immersion.

Remark .1.3. Any neighborhood of M in $\mathcal{G}$ is again a local Lie groupoid by restriction of the structural maps α and β and shrinking of $\mathcal{V}$.

Since what matters in the present appendix lies in any neighborhood of M and using the previous remark, we will assume that the source has connected fibers. Notice that it implies the same property for the target.

Remark .1.4. The local product might be understood as follows. Given $a \in \mathcal{G}$, $a.b$ exists and is in $\mathcal{G}$ if and only if $\beta(a) = \alpha(b)$ and b is sufficiently close to the identity section.

The existence of a local product allows to define invariant vector fields on $\mathcal{G}$.

Definition .1.5. Let $X \in \mathfrak{X}(\mathcal{G})$. X is said to be left invariant (resp. right invariant) if for any $(a, b) \in \mathcal{V}$,

$$X \circ L_a(b) = T_b L_a X(b), \tag{1}$$

respectively

$$X \circ R_b(a) = T_a R_b X(a), \tag{2}$$

where L_a denotes the left translation by a and R_b denotes the right translation by b.

Remark .1.6. Equations (1) and (2) imply respectively that for any $(a, b) \in \mathcal{V}$, if X is left invariant:

$$\Phi_X^t(a \cdot b) = a \cdot \Phi_X^t(b) \tag{3}$$

and if X is right invariant:

$$\Phi_X^t(a \cdot b) = \Phi_X^t(a) \cdot b. \tag{4}$$

Proposition .1.7. *Let X and Y two vector fields on $\mathcal{G}$ such that X is left invariant and Y is right invariant. Then,*

$$[X, Y] = 0 \tag{5}$$

Proof. Using remark .1.6, the flows of X and Y commute: for any $a \in \mathcal{G}$, any $t \in \mathbb{R}$ such that $\Phi_X^t(i(\beta(a)))$ exists and any $s \in \mathbb{R}$ such that $\Phi_Y^s(a)$ exists,

$$\Phi_Y^s \circ \Phi_X^t(a) = \Phi_Y^s(a) \cdot \Phi_X^t(i(\beta(a)) \tag{6}$$

$$= \Phi_X^t \circ \Phi_Y^s(a). \tag{7}$$

□

.1.2 Local symplectic groupoids

Multplicative symplectic structures on local Lie groupoids – in the following sense – allow to study Poisson structures and are used in the present manuscript to study Hamiltonian dynamics on them.

Definition .1.8 (Local symplectic groupoid)**.** $(\mathcal{G}, \Omega)$ is said to be a local symplectic groupoid if $\mathcal{G}$ is a local Lie groupoid equipped with the symplectic form Ω and if Ω is multiplicative:

$$m^*\Omega = (\mathrm{pr}_1)^*\Omega + (\mathrm{pr}_2)^*\Omega, \tag{8}$$

where for $i = 1, 2$, $\mathrm{pr}_i \colon \mathcal{V} \to \mathcal{G} \colon (a_1, a_2) \mapsto a_i$.

Thanks to the multiplicative symplectic form Ω, the musical isomorphism from $T\mathcal{G}$ to $T^*\mathcal{G}$ relates invariant vector fields on $\mathcal{G}$ to pull-back of 1-forms through source and target by the following lemma:

Proposition .1.9. *There is a 1-1 correspondence between:*

- *left (resp right) invariant vector fields on $\mathcal{G}$,*
- *pull-backs of 1-forms on M through the target map (resp. the source map).*

Proof. Let $X \in \mathfrak{X}(\mathcal{G})$ a left invariant vector field and set $\zeta = \Omega(X, .) \in \Omega^1(\mathcal{G})$.

A consequence of the multiplicativity of Ω is the fact that translations are symplectomorphisms. Combining this observation with the left invariance of X:

$$\forall Y \in \mathfrak{X}(\mathcal{G}),\ \forall a \in \mathcal{G},\ \zeta\left((L_a)_* Y\right) = \zeta(Y) \circ L_a, \tag{9}$$

inducing $\zeta \in \mathrm{Im}\left(\beta^* \colon \Omega^1(M) \to \Omega^1(\mathcal{G})\right)$ as a consequence. ζ is unique by non-degeneracy of Ω and that proves the correspondence for left invariant vector fields, the one for right invariance vector fields being proven the same way. □

Remark .1.10. Since T^*M is the algebroid of $\mathcal{G}$, this correspondence might be extended in the more general setting of algebroids, although such generalities are not required for the present manuscript.

Let us introduce the following notations: we will write $\overleftarrow{\xi}$ for the left invariant vector field associated to the 1-form $\zeta \in \Omega^1(M)$ and $\overrightarrow{\xi}$ for the right invariant one. The commuting property between pull-packs and the de Rham differential gives the immediate

Corollary .1.11. *For any Hamiltonian $H \in \mathcal{C}^\infty(M)$, $\overleftarrow{dH}$ is the Hamiltonian vector field of $\beta^* H$ while $\overrightarrow{dH}$ is the Hamiltonian vector field of $\alpha^* H$.*

Let us give a first geometric property of $\mathcal{G}$ seen as a symplectic manifold.

Proposition .1.12. *The identity section i is a Lagrangian embedding of the base space M into the arrow space $\mathcal{G}$.*

Proof. M is isotropic by multiplicity of Ω. Furthermore, the graph of m in $\mathcal{G}^3$ is at the same time of dimension $2\dim\mathcal{G} - \dim M$ by rank-nullity theorem and if dimension $\frac{3}{2}\dim\mathcal{G}$ by (8). □

Lemma .1.13. $\forall (f, g) \in \mathcal{C}^\infty(M)^2,\ \{\alpha^* f, \beta^* g\}_\Omega = 0$.

Proof. Thanks to the corollary .1.11, a proof is given by the following observation that the flow of a left invariant vector field preserves the source. □

This last lemma can be rephrased as follows: the source and target fibers are symplectically dual to each other. It admits an important consequence:

Proposition .1.14. *There exists a unique Poisson structure on M such that the source α is Poisson.*

Proof. Jacobi relation for $\{.,.\}_\Omega$ gives for any $(f, g, h) \in \mathcal{C}^\infty(M)$

$$\{\{\alpha^* f, \alpha^* g\}_\Omega, \beta^* h\}_\Omega = 0. \tag{10}$$

Using lemma .1.13, one obtains that $\{\alpha^* f, \alpha^* g\}_\Omega \in \mathcal{C}^\infty(\mathcal{G})$ is invariant on fibers of α: there exists a smooth function on M such that its pull-back by α is $\{\alpha^* f, \alpha^* g\}_\Omega$. The transformation taking f and g to this smooth function verifies axioms of a Poisson bracket and that concludes the proof. □

.1.3 Lagrangian bisections

Definition .1.15. A submanifold L of $\mathcal{G}$ is a Lagrangian bi-section if:

1. L is Lagrangian,
2. α and β restrict to L as diffeomorphisms from L to M.

Proposition .1.16. *Set $\phi_L = \beta \circ \alpha_{|L}^{-1} \colon M \to M$. ϕ_L is a Poisson automorphism.*

Proof. L induces a symplectomorphism ξ_L of $\mathcal{G}$ by right translations. We set, for any $a \in \mathcal{G}$,

$$\chi_L(a) = a \cdot \alpha_{|L}^{-1} \circ \beta(a). \tag{11}$$

Since L is Lagrangian, $(\chi_L)^*\Omega = \Omega$. Besides, let us observe that the following diagram commute:

$$\begin{array}{ccc} \mathcal{G} & \xrightarrow{\chi_L} & \mathcal{G} \\ {\scriptstyle\beta}\downarrow & & \downarrow{\scriptstyle\beta} \\ M & \xrightarrow{\phi_L} & M \end{array}, \tag{12}$$

from which we obtain, for any f and g in $\mathcal{C}^\infty(M)$,

$$\begin{aligned} \beta^*(\phi_L)^*\{f,g\}_\pi &= (\chi_L)^*\beta^*\{f,g\}_\pi && (13)\\ &= -\{(\beta\xi_L)^*f, (\beta\xi_L)^*g\}_\Omega && (14)\\ &= \beta^*\{(\phi_L)^*f, (\phi_L)^*g\}_\pi && (15) \end{aligned}$$

which concludes by injectivity of $\beta^* \colon \mathcal{C}^\infty(M) \to \mathcal{C}^\infty(G)$. □

Example .1.17. The identity section is a Lagrangian bi-section inducing the identity on M.

Remark .1.18. The set of Lagrangian bisections of $\mathcal{G}$ can be equipped with a group law (see, for instance, [61]). Since the right translation of the product of two Lagrangian bi-sections is the composition of the two translations, the commutativity of the diagram (12) provides the following formula: for L and K two Lagrangian bisections,

$$\phi_{L\cdot K} = \phi_L \circ \phi_K. \tag{16}$$

Proposition .1.19. *Let $H \in \mathcal{C}^\infty(M)$ and t such that the Hamiltonian flow $\Phi^t_{\alpha^*H}$ of α^*H exists. Set $L = \Phi^t_{\alpha^*H}(M)$. Then:*

1. *L is a Lagrangian bi-section,*
2. *it induces $\phi_L = \Phi^t_H$ on M.*

Proof. L is a Lagrangian submanifold because $\Phi^t_{\alpha^*H}$ is a symplectomorphism. Let us show that it is a bi-section.

Let $x \in M$ and let us show that there exists a unique $a \in L$ such that $\beta(a) = x$. From lemma .1.13, we obtain

$$\beta \circ \Phi^t_{\alpha^*H} = \beta \tag{17}$$

and so $a = \Phi^t_{\alpha^*H}(i(x))$ suits. It is unique by (17).

Let us show that there exists a unique $a \in L$ such that $\alpha(a) = x$. Since $X_{\alpha^* H} = \overrightarrow{\mathrm{d}H}$, applying (4) to $\overrightarrow{\mathrm{d}H}$:

$$\mathrm{inv}\left(\Phi^t_{\alpha^* H}(M)\right) = \Phi^{-t}_{\alpha^* H}(M) \tag{18}$$

Since $\alpha = \beta \circ \mathrm{inv}$, a similar argument as the one used for β above allows to conclude that L is indeed a Lagrangian bi-section.

We are left to prove that $\phi_L = \Phi^t_H$. Let f be a smooth function on M. Thanks to the diagram (12):

$$\beta^* \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} f \circ \phi_L = \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} f \circ \beta \circ \chi_L \tag{19}$$

$$= -\{\beta^* f, \beta^* H\}_\Omega. \tag{20}$$

We conclude by anti-Poisson and surjectivity properties of β. □

.1.4 Local product of a bi-realisation

This theorem is proved in chapter III of [16], pages 37-44.

Theorem .1.20. *Let $\mathcal{U}$ a tubular neighborhood of M in T^*M equipped with the canonical symplectic form ω and α and β two surjective submersions from $\mathcal{U}$ to M such that:*

1. *α and β are respectively Poisson and anti-Poisson,*
2. *for every f and g in $\mathcal{C}^\infty(M)$, $\{\alpha^* f, \beta^* g\} = 0$,*
3. *α and β are left inverses of the identity section, meaning $\alpha_{|M} = \beta_{|M} = id_M$.*

Then, there exists a tubular neighborhood $\tilde{\mathcal{U}} \subset \mathcal{U}$ on which a local product is defined. This local product induces on $\tilde{\mathcal{U}}$ the structure of a local symplectic groupoid over M.

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