Abstract

In this article we introduce a new method for constructing implicit symplectic maps using special symplectic manifolds and Liouvillian forms. This method extends, in a natural way, the method of generating functions to 1-forms which are globally defined on the symplectic manifold. The maps constructed by this method, are related to the symplectic Cayley’s transformation and belong to a continuous space of dimension $n(2n+1)$. Applying the implicit map to the discrete Hamilton equations we obtain the generalized symplectic Euler scheme. We show the relations of the elements of this family with other discrete symplectic mappings, in particular 1) with the mappings obtained by generating functions of type I, II, and III and IV; 2) with the symplectic Euler methods A and B; and 3) with the mid-point rule. Moreover, we show the corresponding symplectic diffeomorphisms and their Liouvillian forms on the product symplectic manifold. We illustrate the details of the method in constructing two different families of implicit symplectic maps for $n = 1$. This is a geometrical method which overcomes the difficulties of the Hamilton-Jacobi theory and generating functions.

1 Introduction

Symplectic maps can be constructed by using generating functions, and they were introduced by Poincaré when looking for periodic orbits of second genus [10]. From the numerical point of view, symplectic maps are used for simulating Hamiltonian dynamics, based on the fact that the Hamiltonian flow is a one parameter subgroup of symplectic diffeomorphisms. In the classical construction of symplectic maps, the use of Darboux’s coordinates in different stages of the procedure hides several interesting properties, which arise with the discretization in time of Hamiltonian flows. Other properties do not appear in the

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continuous case due to a classical procedure of reduction from symplectic to contact geometry, which takes the Hamiltonian vector field into the Reeb field on the reduced manifold [8, 7].

In this paper, we address the problem of constructing implicit symplectic maps with a different approach. Instead of using Hamilton-Jacobi theory to obtain a generating function, we take advantage of the geometrical properties of both the Hamiltonian flow and the product symplectic manifold. However, we avoid the use of Darboux’s theorem and the classical evolutive Hamilton-Jacobi equation. The reason is that the coordinates of the original problem are locally conjugated to the canonical coordinates by a symplectomorphism which is hidden by Darboux’s theorem. In consequence, the classical construction integrates a modified problem in normal form using action-angle coordinates. Instead of Darboux’s theorem we use special symplectic manifolds [14, 13, 12] and their Liouvillian forms in order to track the state of the original coordinates at every stage of the procedure.

This approach differs from the standard procedure of generating functions in two ways. First, we consider Lagrangian submanifolds as the integral submanifolds of a prescribed Liouvillian form \( \theta \) [8, 7], i.e. submanifolds defined by the differential ideal \( I \) generated by \( \theta \). Second, we use the complex structure on the product manifold to obtain the equations of the tangent space to the Lagrangian submanifold defined implicitly by the Liouvillian form. The advantage in the symplectic case is that the vertical bundle corresponds to the characteristic bundle to the Lagrangian submanifold. In our method, the Liouvillian form substitutes the generating function and the multiplication with the complex structure on the product manifold substitutes the role of the resolution of the Hamilton-Jacobi equation. An additional projection of the Lagrangian submanifold offers the possibility to construct symplectic maps by a simple transversality condition. For the linear case, this condition is weakened by the classical condition stating that the symplectic map must converge to the identity map on the diagonal of the product manifold. All this procedure is constructed on the framework of special symplectic manifolds.

The latter condition is translated into a condition relating two different Liouvillian forms on the original symplectic manifold. Surprisingly, using this relation, the framework of special symplectic manifolds is no more necessary. In this way, we can construct symplectic maps just using Liouvillian forms, leading to the method of Liouvillian forms. This procedure reveals some remarkable properties and gives a different perspective on Liouvillian forms and generating functions. We give an interpretation of this method as a discrete version of the Cayley’s transformation of a Hamiltonian matrix, leading naturally to a symplectic map. Finally, we construct a numerical scheme, which is the natural generalization of the Euler symplectic schemes.

We summarize the rest of the paper. In Section 2 we give the main definitions and classical results on symplectic manifolds and the product manifold that are necessary for our exposition. Special symplectic manifolds and Liouvillian forms are exposed in Section 3. In this section we introduce the generating functions of type I, II, III and IV and their related Liouvillian forms expressed
as elements of some special symplectic manifolds. We return systematically to these examples in the rest of the paper. In Section 4 we expose the way we can construct symplectic maps using Liouvillian forms. Section 5 gives the structure of Liouvillian forms on the symplectic manifold and the product symplectic manifold. In Section 6 we construct the implicit map. Section 7 describes all four steps of the method of Liouvillian forms and we state our main result. In addition, we relate these maps to the symplectic Cayley’s transformation. In Section 8 we apply the implicit maps to Hamiltonian dynamics and we introduce the generalized implicit symplectic Euler scheme. We show that the mid-point rule, and the symplectic Euler A and B maps are particular cases of our scheme. Finally, in Section 9 we develop two examples of continuous families of implicit symplectic integrators: the first one using special symplectic manifolds and the second one applying the generalized symplectic Euler scheme.

2 Symplectic manifolds and symplectic mappings

In this section we recall some classical results and definitions in order to uniformize the notation. The results are stated in a geometrical fashion in preparation of the next section where we will set the framework of the method of Liouvillian forms. We assume the reader is familiar with the terminology of differential geometry and vector bundles. For an introduction the reader is referred to [1, 8, 9].

A symplectic manifold is a $2n$-dimensional manifold $M$ equipped with a non-degenerated, skew-symmetric, closed 2-form $\omega$, such that at every point $m \in M$, the tangent space $T_mM$ has the structure of a symplectic vector space. In addition, we say that $(M,\omega)$ is an exact symplectic manifold if there exists a 1-form $\theta$ such that $\omega = d\theta$; $\theta$ is called a Liouvillian form. In what follows, all the symplectic manifolds will be exact.

An almost complex structure $J$ on a manifold $M$ is a smooth tangent bundle isomorphism $J : TM \to TM$ covering the identity map on $M$ such that for each point $z \in M$, the map $J_z = J(z) : T_zM \to T_zM$ is a complex structure on the vector space $T_zM$, it means an endomorphism on $T_zM$ such that $J^2(v) = J \circ J(v) = -v$ for every $v \in T_zM$. We write $J^2 = -I$ for simplicity. A symplectic manifold with an almost complex structure possesses a Riemannian structure $g$ which enables the definition of a symmetric positive definite form where $\omega(\cdot,\cdot) = g(\cdot, J \cdot)$. We fix the Riemannian structure $g(\cdot, \cdot) = \langle \cdot, \cdot \rangle$ such that at every point on any symplectic manifold $x \in M$, the tangent space $(T_xM, \langle \cdot, \cdot \rangle_x)$ is an inner product space.

A submanifold $\Lambda \subset M$ is called Lagrangian if the symplectic form restricted to $\Lambda$ vanish $\omega|_{\Lambda} \equiv 0$. The tangent bundle to the symplectic manifold $TM$ splits into the tangent $TA$ and the vertical $VA$ bundles of the Lagrangian submanifold in the form $TM = TA \oplus VA$, where $VA := (TA)^\perp$ is the complementary subbundle to $TA$. The complex structure $J$ and the non degeneracy of $\omega$ on $M$, let us rewrite the vertical bundle as $V_x\Lambda = JT_x\Lambda$ for every $x \in \Lambda$. We write
Let \((M, \omega)\) be a symplectic manifold. A diffeomorphism \(f : M \to M\) is said symplectic or a symplectomorphism if \(f^* \omega = \omega\), where \(f^*\) denotes the pullback of the 2-form defined by

\[
(f^* \omega)_z(u, v) = \omega_{f(z)}(Tf(u), Tf(v)), \quad z, f(z) \in M, u, v \in T_z M.
\]

In this expression \(Tf : TM \to TM\) is the tangent map of \(f : M \to M\). The set of all the symplectic diffeomorphisms on a symplectic manifold form a group denoted by \(Sp(M, \omega)\) and called the symplectic group of \((M, \omega)\).

In order to construct symplectic maps we follow the classical construction. Define the product manifold of two copies of an exact symplectic manifold \((M, \omega)\) at times \(t = 0\) and \(t = h\), which we denote by \((M_1, \omega_1)\) and \((M_2, \omega_2)\), respectively. The manifold \(\tilde{M} = M_1 \times M_2\) with the canonical projections \(\pi_i : \tilde{M} \to M_i\) for \(i = 1, 2\) let us define the forms \(\theta \ominus\) and \(\omega \ominus\) on \(\tilde{M}\) by

\[
\theta \ominus = \pi_1^* \theta_1 - \pi_2^* \theta_2, \quad \omega \ominus = \pi_1^* \omega_1 - \pi_2^* \omega_2
\]

We have the following facts (see [1, sec 5.2] for the proofs):

- \((\tilde{M}, \omega \ominus)\) is a symplectic manifold of dimension \(4n\).
- For any symplectic map \(\phi : M_1 \to M_2\), the graph of \(\phi\), denoted by \(\Lambda_\phi\), and defined by
  \[
  \Lambda_\phi = \{(z, \phi(z)) \in \tilde{M} \mid z \in M_1, \phi(z) \in M_2\}
  \]
  is a Lagrangian submanifold of \(\tilde{M}\). It means \(\omega \ominus|_{\Lambda_\phi} = 0\).
- Since \(\omega \ominus = d\theta \ominus\), then \(\theta \ominus\) is a locally closed form on \(\Lambda_\phi\). Applying Poincare’s lemma, \(\theta \ominus\) is locally exact in a neighborhood of \(\Lambda_\phi\). Consequently, there exists a function \(S\) defined on the Lagrangian submanifold \(\Lambda_\phi\) such that its differential coincides with the restriction of the 1-form \(\theta \ominus\) to \(\Lambda_\phi\). It means that
  \[
  dS|_{\Lambda_\phi} = \theta \ominus|_{\Lambda_\phi}
  \]
  The function \(S : \Lambda_\phi \to \mathbb{R}\) is called a generating function for the symplectic map \(\phi\).
- There exists and induced endomorphism on \(T_\phi \tilde{M}\) which becomes the associated complex structure on \(\omega \ominus\) given by
  \[
  \tilde{J} = (T\pi_1)^T J_1 - (T\pi_2)^T J_2
  \]
  where \(J_i\) are the associated complex structures to \(\omega_i, i = 1, 2\).
Symplectic maps, generating functions, Liouvillian forms and Lagrangian submanifolds are closely related. For instance, in a generic symplectic manifold $M$, any Lagrangian submanifold $\Lambda \subset M$ which is transverse to the fibers of the projection $\pi_M : T^*M \to M$ can be parameterized by a suitable (local) function $S$. In contrast, Liouvillian forms are globally defined and they do not need a particular parameterization, however topological properties of the underlying manifold like characteristic classes prevent the use of these forms in particular applications.

We rephrase some classical properties of Lagrangian and symplectic submanifolds in term of the symplectic product manifold $\tilde{M}$.

Lemma 2.1 Let $\Lambda \subset \tilde{M}$ be a Lagrangian submanifold and $\Phi \in \text{Sp}(\tilde{M}, \omega_{\otimes})$ a symplectomorphism. We have the following facts:

1. The image of the Lagrangian submanifold under $\Phi$ is again a Lagrangian submanifold of $M$.

2. The projection $\pi_i(\Lambda) \subset M_i$ is a Lagrangian submanifold in $M_i$, $i = 1, 2$.

Proof. 1) Let $\tilde{\Lambda} = \Phi(\Lambda)$ be the image of $\Lambda$ under the symplectomorphism $\Phi$. For all $y \in \tilde{\Lambda}$ and $\xi, \eta \in T_y \tilde{\Lambda}$ there exist $x \in \Lambda$ and $u, v \in T_x \Lambda$ such that $y = \Phi(x)$, $\xi = T\Phi(u)$ and $\eta = T\Phi(v)$. Since $\Phi^*\omega_{\otimes} = \omega_{\otimes}$ we have

$$\langle (\omega_{\otimes})_y(\xi, \eta) = (\omega_{\otimes})_x(u, v) = 0$$

and $\tilde{\Lambda}$ is a Lagrangian submanifold in $(\tilde{M}, \omega_{\otimes})$.

2) Since $\tilde{M} = M_1 \times M_2$ is a product manifold, its tangent bundle splits into $T\tilde{M} = TM_1 \oplus TM_2$. The subbundle $T\Lambda \subset T\tilde{M}$ is given under the splitting by $T\Lambda = TA_1 \oplus TA_2$. We have $T\pi_i(T\Lambda) = T\Lambda_i \subset TM_i, i = 1, 2$. Due to the splitting $T\Lambda = TA_1 \oplus TA_2$ then $\omega_{\otimes}\mid\Lambda \equiv 0$ if and only if $\omega_{\otimes}\mid\pi_i(\Lambda) \equiv 0$ and consequently $\pi_i(\Lambda) \subset M_i$ are Lagrangian submanifolds for $i = 1, 2$. □

Lemma 2.2 Let $\phi_i \in \text{Sp}(M_i, \omega_i), i = 1, 2$ be two symplectomorphisms. The induced diffeomorphism on $\tilde{M}$ by diagonal action on $M_1 \times M_2$ defined by $\Phi(\tilde{M}) = \phi_1(M_1) \times \phi_2(M_2)$, is a symplectic diffeomorphism in $\tilde{M}$.

Proof. It is enough to show that $\Phi^*\omega_{\otimes} = \omega_{\otimes}$. By definition of the symplectic form and the fact that $\phi_i, i = 1, 2$ are symplectomorphisms we have

$$\omega_{\otimes} = \pi_1^*\omega_1 - \pi_2^*\omega_2 = \pi_1^* \circ \phi_1^* \omega_1 - \pi_2^* \circ \phi_2^* \omega_2 = (\phi_1 \circ \pi_1)^* \omega_1 - (\phi_2 \circ \pi_2)^* \omega_2.$$

Applying the properties of the pull-back of the composition we obtain

$$\omega_{\otimes} = (\phi_1 \circ \pi_1)^* \omega_1 - (\phi_2 \circ \pi_2)^* \omega_2 = \Phi^*\omega_{\otimes}$$

which gives the result. □

This last result gives us the possibility to consider Lagrangian submanifolds which do not look like the graph of a diffeomorphism in $\tilde{M}$. It lets us work with Lagrangian submanifolds in mixed coordinates, or in other words with generic implicit symplectic mappings.
3 Special symplectic manifolds and Liouvillian forms

An important class of symplectic manifolds are the cotangent bundle to Riemannian manifolds. In particular, they model the phase space of many Hamiltonian mechanical systems, where the base coordinates correspond to positions or configurations, and vertical coordinates correspond to momenta.

Let $Q$ be a $C^\infty$ manifold. Consider the cotangent and tangent bundles $T^*Q$ and $TQ$, and its canonical projections on the base manifold $Q$ denoted by $\tau_Q : TQ \to Q$ and $\pi_Q : T^*Q \to Q$ respectively.

The projection $\pi_Q$ determines a natural map between the cotangent bundle and the double cotangent bundle by its pullback $\pi_Q^* : T^*Q \to T^*(T^*Q)$, which sends 1-forms on $Q$ to 1-forms on $T^*Q$ by $\theta = \pi_Q^* \eta$ for every 1-form $\eta$ defined on $Q$. Formally $\eta$ is a section of the cotangent bundle that we denote by $\eta \in \Gamma(T^*Q)$, where $\Gamma(T^*Q)$ denotes the space of smooth sections on the cotangent bundle.

The form $\theta = \theta_\eta$, induced by the identity morphism $\theta_\eta = (\pi_Q^*)_\eta(\eta)$ for every $\eta \in \Gamma(T^*Q)$, is called the Liouville form on $T^*Q$ and is alternatively defined by its action on the tangent bundle by the equation

$$\langle v, \theta_\eta \rangle_{T^*Q} = \langle T\pi_Q(v), \eta \rangle_Q, \quad v \in T_\eta T^*Q, \quad \eta \in \Gamma(T^*Q), \quad \theta_\eta \in T^*_\eta(T^*Q).$$

Remark 1 The double cotangent bundle $(T^*(T^*Q), T^*Q, \pi_{T^*Q})$ is defined by the projection $\pi_{T^*Q} : T^*(T^*Q) \to T^*Q$. Consequently, the canonical Liouville form

\footnote{We use the notation $\beta \in \Gamma E$ instead of $\beta \in \Gamma(E)$ for simplifying the notation in the diagrams.}
form $\theta \in \Gamma(T^*(T^*Q))$ is a section in $T^*(T^*Q)$ corresponding to the inclusion of sections from $\Gamma(T^*Q)$ into $\Gamma(T^*(T^*Q))$. This inclusion is also interpreted as the identity map. The fact that the Liouville form is a section of the double cotangent bundle is not evident when we work with symplectic vector spaces and it has been the source of many misunderstandings in some areas like the numerical analysis.

When we shall have the occasion to deal with cotangent bundles of different manifolds, we will denote the Liouville form on $T^*N$ by $\theta_N$.

The cotangent bundle $T^*Q$ inherits a natural symplectic structure $\omega = d\theta_Q$ such that the couple $(T^*Q, \omega)$ becomes a symplectic manifold. Unfortunately, many geometrical properties of symplectic manifolds lost significance in mechanical systems due to a missing physical interpretation. Tulczyjew proposed in [14] the study of symplectic manifolds which are diffeomorphic to cotangent bundles by means of special symplectic manifolds (see also [13, 12]).

A special symplectic manifold is a quintuple $(M, \theta, \pi, \varphi)$ where $\pi: M \to Q$ is a fibre bundle, $\theta$ is a 1-form on $M$ and $\varphi: M \to T^*Q$ is a symplectic diffeomorphism such that $\pi = \pi_Q \circ \varphi$, and $\theta = \varphi^*\theta_Q$.

The pair $(M, d\theta)$ is a symplectic manifold. We call the 1-form $\theta = \varphi^*\theta_Q$ a Liouvillian form on $M$. More generally we say that a 1-form $\eta$ on an even dimensional symplectic manifold $(M, \omega)$ is Liouvillian or of Liouvillian type if $d\eta$ is a symplectic form on $M$, or equivalently if $(M, d\eta)$ is a symplectic manifold.

Let $K \subset Q$ be a submanifold and $S: K \to \mathbb{R}$ a function on $K$. The Lagrangian submanifold generated by $S$ in the manifold $(M, d\theta)$ is defined by the equation $\langle v, \theta \rangle = \langle T\pi(v), dS \rangle$ where $v \in TM$ and $\tau_M(v) = m$, in the following way

$$\Lambda = \{ m \in M | \pi(m) \in K, \langle v, \theta \rangle = \langle T\pi(v), dS \rangle \}. \tag{4}$$

We suppose $K \subset Q$ is an embedded submanifold and we write it as an inclusion $i: K \to Q$. In this case $i^*(dS) \in \Gamma(T^*K)$ and $dS \in \Gamma(T^*Q)$. If in addition, we suppose that $i: K \to Q$ is an immersion, $\pi$ defines a submersion

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Libermann and Marle [8] and Libermann [7] define Liouvillian forms in the more general context of bundle morphisms. We use a simplified definition for working with special symplectic manifolds.
and the submanifold $\Lambda$ is well defined. The following graph shows this situation

Any special symplectic manifold $(M, Q, \theta, \pi, \varphi)$ determines a natural splitting of the tangent bundle $TM = T\Lambda \oplus VA$ using the Liouvillian form $\theta = \varphi^* \theta_Q$ and the projection $\pi = \pi_Q \circ \varphi$. The projection keeps track of the deformation of the tangent (horizontal) bundle, and the Liouvillian form recovers the deformation of the vertical bundle.

The following result relates the symplectic manifolds of interest in this work: $(\tilde{M}, \omega \ominus) \text{ and } (T^* (Q_1 \times Q_2), d\theta_Q \times Q_2)$, where $\theta_Q \times Q_2$ is the Liouville form on $Q_1 \times Q_2$.

**Proposition 1** Define coordinates $(q, p, Q, P) \in \tilde{M}$ in the product manifold such that $(q, p) \in M_1$ and $(Q, P) \in M_2$. Let $E_1 : \tilde{M} \to T^* (Q_1 \times Q_2)$ be the linear map given by

$$E_1 : \tilde{M} \to T^* (Q_1 \times Q_2)$$

$$(q, p, Q, P) \mapsto (q, -Q, p, P).$$

(5)

Then $E_1$ is a symplectomorphism.

**Proof.** Define coordinates $(x, X, y, Y) \in T^* (Q_1 \times Q_2)$ where $(x, X) \in Q_1 \times Q_2$. We have $(x, X, y, Y) = (q, -Q, p, P)$ and the Liouville form in these coordinates becomes $\theta_{Q_1 \times Q_2} = y dx + dX$. Taking the differential we have

$$E_1^* (dy \wedge dx + dY \wedge dX) = dp \wedge dq - dP \wedge dQ = \omega \ominus$$

as we want to show. □

$E_1$ is known as the canonical symplectomorphism between the product manifold $(\tilde{M}, \omega \ominus)$ and the cotangent bundle $(T^* (Q_1 \times Q_2), d\theta_Q \times Q_2)$.

**Corollary 1** Let $\Phi \in Sp(\tilde{M}, \omega \ominus)$ be a symplectomorphism on $\tilde{M}$ and consider $E_1$ as below. Then the diffeomorphism $\Psi : \tilde{M} \to T^* (Q_1 \times Q_2)$ given by

$$\Psi = E_1 \circ \Phi$$

(6)
is symplectic.

**Proof.** Direct from the fact that \( \Psi : \tilde{M} \to T^*(Q_1 \times Q_2) \) is the composition of two symplectomorphisms

\[
\begin{array}{c}
\tilde{M} \\
\Phi \\
\downarrow \\
\Psi \\
\downarrow \\
\tilde{M} \\
\end{array} \quad \begin{array}{c}
\Phi \\
\downarrow \\
\Psi \\
\downarrow \\
T^*(Q_1 \times Q_2). \\
\end{array}
\]

The quintuple \((\tilde{M}, Q_1 \times Q_2, \theta, \pi, \Psi)\), where \( \Psi \) is defined in (6) becomes a special symplectic manifold on \( Q_1 \times Q_2 \).

We recall that any Lagrangian submanifold \( \Lambda \subset T^*(Q_1 \times Q_2) \) defines a Lagrangian submanifold in \( \tilde{M} \) by the symplectomorphism \( \Psi^{-1}(\Lambda) \).

### 3.1 Examples of special symplectic manifolds

We consider some simple symplectomorphisms between the product of two symplectic manifolds and the cotangent to the product of two configuration spaces \( \tilde{M} \to T^*(Q_2 \times Q_1) \). These symplectomorphisms define four special symplectic manifolds and we will be interested in their Liouvillian forms. Using symplectic coordinates on the manifolds \((x_i, X_i, y_i, Y_i) \in T^*(Q_1 \times Q_2)\) and \((q_i, p_i, Q_i, P_i) \in \tilde{M}\) we consider four symplectic diffeomorphisms

1. \( E_1(q_i, p_i, Q_i, P_i) = (q_i, -Q_i, p_i, P_i) \) corresponding to the canonical symplectic diffeomorphism from \( \tilde{M} \to T^*(Q_2 \times Q_1) \). The Liouville form on \( T^*(Q_2 \times Q_1) \) corresponding to \( \theta_{Q_1 \times Q_2} \) is pulled back to the Liouville form \( \theta = (E_1^*)\theta_{Q_1 \times Q_2} \) and it corresponds to the form \( \theta_{\tilde{M}} \) on \( \tilde{M} \). For instance, the Liouvilian form and the projection are
   \[
   \theta_{\tilde{M}} = p_i dq_i - P_i dQ_i \quad \text{and} \quad \pi(q_i, p_i, Q_i, P_i) = (q_i, -Q_i).
   \]

2. \( \Psi_{11}(q_i, p_i, Q_i, P_i) = (q_i, P_i, p_i, Q_i) \). This diffeomorphism gives the Liouvillian form and projection given by
   \[
   \theta = p_i dq_i + Q_i dP_i \quad \text{and} \quad \pi(q_i, p_i, Q_i, P_i) = (q_i, P_i).
   \]
3. \(\Psi_{III}(q_i, p_i, Q_i, P_i) = (Q_i, p_i, -P_i, -q_i)\). This diffeomorphism gives the following Liouvillian form and projection
\[
\theta = -q_idp_i - P_idQ_i \quad \text{and} \quad \pi(q_i, p_i, Q_i, P_i) = (Q_i, p_i).
\]

4. \(\Psi_{IV}(q_i, p_i, Q_i, P_i) = (-p_i, P_i, q_i, Q_i)\). This diffeomorphism gives the following Liouvillian form and projection
\[
\theta = -q_idp_i + Q_idP_i, \quad \text{and} \quad \pi(q_i, p_i, Q_i, P_i) = (-p_i, P_i).
\]

Since the Liouvillian form on \(\tilde{M}\) corresponds to a class of symplectomorphisms modulo symplectic rotations we need both elements, the Liouvillian form and the projection for fixing the symplectomorphism between these manifolds. The symplectomorphisms \(E_1, \Psi_{II}, \Psi_{III}, \Psi_{IV}\) will be revisited in the next section where we related them to generating functions.

4 Symplectic maps from Liouvillian forms

The usual way to construct symplectic maps on the product manifold \((\tilde{M}, \omega_{\otimes})\) is using generating functions \(S : \Lambda \to \mathbb{R}\) defined on some Lagrangian submanifold \(\Lambda \subset \tilde{M}\); it is an inverse problem. This inverse problem is solved using Hamilton-Jacobi theory for estimating the characteristic bundle which contains, as a subbundle, the vertical bundle to the Lagrangian submanifold. We deal with this problem in a more direct way using Liouvillian forms which define Lagrangian submanifolds as their integral submanifolds. The transformation between the vertical and the tangent bundles is given by the complex structure associated to the symplectic form. In this way we avoid the solution of both the Hamilton-Jacobi equation and the generating function. However, in both procedures, we must select what type of symplectic maps we are looking for. In our case, we are interested on symplectic maps adapted for constructing numerical schemes which differ from those used for studying periodic orbits in an essential way. The task in this section is to characterize Lagrangian submanifolds adapted for constructing numerical schemes.

Remark 2 Symplectic maps for numerical schemes and those used for studying periodic orbits solve variational problems with different boundary conditions. The former consider the minimization of the action integral along paths joining two different fixed points; the latter consider closed paths with prescribed period \(T > 0\). This implies that Poincaré’s differential form\(^3\) introduced in \([10]\) for studying bifurcations of periodic orbits is not well suited for constructing numerical schemes. A detailed study of this fact is given in \([4]\).

To obtain a symplectic map for constructing numerical schemes we need to recover a symplectic vector space from the information encoded in the tangent

\(^3\)It is the differential of the so called Poincaré’s generating function
space to the Lagrangian submanifold $\Lambda \subset \tilde{M}$. In fact, we state a stronger condition. Let $(\tilde{M}, Q_1 \times Q_2, \theta, \pi, \Psi)$ be the special symplectic manifold defined in the last section and consider the image $N = \pi(M)$ of the projection $\pi = \pi_{Q_1 \times Q_2} \circ \Psi$ as a submanifold by the adapted inclusion $i : N \hookrightarrow \tilde{M}$. If we can give a symplectic structure $\omega_N$ on $N$ such that $\omega_N = (\pi^*)\omega_{\tilde{M}}$, and $\omega_N = (i^*)\omega_{\tilde{M}}$ then the integral submanifolds of the Liouvillian form $\theta$ on $(\tilde{M}, \omega_{\tilde{M}})$ are adapted for the construction of symplectic integrators.

If the symplectic submanifold $N \subset \tilde{M}$ belongs to a symplectic path joining $z(t) \in M_1 \times M_2$ to $z(t + h) \in M_1 \times M_2$, then the submanifold $(N, \omega_N)$ must converge to the original symplectic manifold

$$\lim_{h \to 0} (N, \omega_N) = (M_1, \omega_1) = (M_2, \omega_2).$$

(7)

We summarize these requirements in the following:

**Condition 1** Consider the tangent space to the projected manifold at a point $\pi(x) \in N, x \in \tilde{M}$, given by $T_{\pi(x)}N = T\pi(T_x\tilde{M})$. Denote by $x \in \Delta \subset \tilde{M}$ a point on the diagonal of the product manifold. If

1. the restriction of $\omega_{\tilde{M}}$ to the submanifold $N = \pi(M)$ is a symplectic form on $N$, and,

2. $T\pi \left( T_x\tilde{M} \right) \bigg|_{x=x} = id$, is the identity,

the Liouvillian form $\theta$ of the special symplectic manifold $(\tilde{M}, Q_1 \times Q_2, \theta, \pi, \Psi)$ defines a Lagrangian submanifold adapted for the construction of a symplectic scheme.

Instead of recovering the symplectomorphism $\Psi$ which defines the special symplectic manifold, we use the fact that Lagrangian submanifolds are the integral submanifolds to Liouvilian forms. Let $\theta_1$ be a Liouvilian form on the $2n$-dimensional symplectic manifold $(M, \omega)$. For every symplectomorphism $\phi : M \rightarrow M$, the form $\theta_2$ given by the pullback $\theta_1 = \phi^*\theta_2$ is again Liouvilian on $(M, \omega)$. They are different Liouvilian forms producing the same symplectic structure $\omega = d\theta_1 = d\theta_2$ on $M$. On the product manifold $(\tilde{M}, \omega_{\tilde{M}})$, the form $\theta = \pi_1^*\theta_1 - \pi_2^*\theta_2$ is Liouvilian on $\tilde{M}$ since $d\theta = \omega_{\tilde{M}}$.

Using point 2) in Lemma 2.1 and Condition 1, we will induce the Liouvilian form on the product manifold $(\tilde{M}, \omega_{\tilde{M}})$ by Liouvilian forms $\theta_1$ and $\theta_2$ on the original symplectic manifold $(M, \omega)$ defining complementary Lagrangian submanifolds. For this, we consider the complex structure $J$ associated to $\omega$.

There exists a (tautological) symplectomorphism $J : M \rightarrow M$ such that its tangent map is exactly the complex structure $TJ = J : TM \rightarrow TM$. This symplectomorphism is attached to every $\omega$.

**Theorem 4.1** For every exact symplectic manifold $(M, \omega)$, there exists at least a Liouvilian form $\theta_1$ on the original symplectic manifold $(M, \omega)$ such that the Liouvilian form

$$\theta = \pi_1^*\theta_1 - \pi_2^*\theta_2, \quad \theta_1 = J^*(\theta_2),$$

(8)
on the product manifold \((\tilde{M}, \omega_{\otimes})\) satisfies Condition 1.

We need additional elements for proving this theorem which follows from Lemma 5.2 below. For the moment, we will relate the Liouvillian forms of the examples given in section 3.1 with the classical generating functions.

**Lemma 4.2** The Liouvillian form of the symplectomorphisms \(E_1, \Psi_{\text{I}}, \Psi_{\text{II}}, \Psi_{\text{IV}}\) given in section 3.1 are associated to the generating functions of type I, II, III and IV, respectively.

**Proof.** We perform the same computations for every symplectomorphism using the Liouvillian form \(\theta\) on the product manifold \((\tilde{M}, \omega_{\otimes})\) and the projection \(\pi = \pi_{(Q_1, Q_2)} \circ \Psi\) for the corresponding \(\Psi\).

1. \(E_1\) produces the Liouvillian form \(\theta = p_i dq_i - P_i dQ_i\), which is locally equivalent to the differential of a function \(S: \tilde{M} \rightarrow \mathbb{R}\) with \(S = S(q_i, Q_i)\) which is a generating function of type I. It defines a Lagrangian submanifold in \(\tilde{M}\) by
   \[
   \Lambda = \{(\hat{q}_i, \hat{p}_i, \hat{Q}_i, \hat{P}_i) \in \tilde{M} | p_i = \frac{\partial S}{\partial q_i}, P_i = -\frac{\partial S}{\partial Q_i}\}.
   \]
   It does not produce a map adapted for constructing symplectic integrators since the projection \(\pi(q_i, p_i, Q_i, P_i) = (q_i, -Q_i)\) does not give symplectic coordinates.

2. \(\Psi_{\text{I}}\) gives the Liouvillian form \(\theta = p_i dq_i + Q_i dP_i\), which is locally equivalent to the differential of a function \(S = S(q_i, P_i)\), which is of type II. It defines a Lagrangian submanifold in \(\tilde{M}\) by
   \[
   \Lambda_{\text{I}} = \{(\hat{q}_i, \hat{p}_i, \hat{Q}_i, \hat{P}_i) \in \tilde{M} | p_i = \frac{\partial S}{\partial q_i}, Q_i = -\frac{\partial S}{\partial P_i}\}.
   \]
   This Liouvillian form is adapted for constructing a symplectic integrator since the projection \(\pi(q_i, p_i, Q_i, P_i) = (q_i, P_i)\) gives symplectic coordinates in the diagonal.

3. \(\Psi_{\text{II}}\) produces the Liouvillian form \(\theta = -q_i dp_i - P_i dQ_i\) which is locally equivalent to the differential of a function \(S = S(Q_i, p_i)\), which is of type III. It defines a Lagrangian submanifold in \(\tilde{M}\) by
   \[
   \Lambda_{\text{II}} = \{(\hat{q}_i, \hat{p}_i, \hat{Q}_i, \hat{P}_i) \in \tilde{M} | q_i = -\frac{\partial S}{\partial p_i}, P_i = -\frac{\partial S}{\partial Q_i}\}.
   \]
   This Liouvillian form is adapted for constructing a symplectic integrator since the projection \(\pi(q_i, p_i, Q_i, P_i) = (Q_i, p_i)\) gives symplectic coordinates in the diagonal.

4. \(\Psi_{\text{IV}}\) gives the Liouvillian form \(\theta = -q_i dp_i + Q_i dP_i\) which is locally equivalent to the differential of a function \(S = S(p_i, P_i)\), which is of type IV. It defines a Lagrangian submanifold in \(\tilde{M}\) by
   \[
   \Lambda_{\text{IV}} = \{(\hat{q}_i, \hat{p}_i, \hat{Q}_i, \hat{P}_i) \in \tilde{M} | q_i = -\frac{\partial S}{\partial p_i}, Q_i = -\frac{\partial S}{\partial P_i}\}.
   \]
This Liouvillian form is not adapted for constructing a symplectic inte-
egrator since the projection \( \pi(q_i, p_i, Q_i, P_i) = (-p_i, P_i) \) does not give 
symplectic coordinates.

5 Structure of Liouvillian forms

Generating functions for constructing symplectic maps are those of type II and I
III, which is not the case for generating functions of type I and IV. This happens 
in the same way for Liouvillian forms. In this section we study the structure of Liouvillian forms for characterizing those adapted for constructing implicit 
symplectic integrators. We recall some facts about the Liouvillian forms on a 
generic exact symplectic manifold \((M, \omega)\).

5.1 Liouvillian forms on an exact symplectic manifold

Consider an exact symplectic manifold \((M, d\theta)\), where \(\theta\) is a generic Liouvillian 
form. For every function \(F: M \to \mathbb{R}\) on \(M\) the differential form \(\theta + dF\) is 
again a Liouvillian form since \(d(\theta + dF) = \omega\). It means, the set of Liouvillian 
forms is invariant under the addition of exact 1-forms. This comes from the fact 
that \(d^2(F)\) corresponds to a symmetric tensor \(S = \text{Hess}(F)\). This generic fact 
implies that the space of Liouvillian forms is infinite-dimensional.

For studying the structure of Liouvillian forms, we want to understand the 
structure of the symplectic form in a generic basis. Given local coordinates 
\(z = (z_i)_{i=1}^{2n} \in M\), a basis of \(T^*_z M \cong \Omega^1(M, \omega)\) is given by 
\(dz_i = \{dz_i\}_{i=1}^{2n}\), and a basis of \(T_z M \cong \Lambda^1(M, \omega)\) is given by \(\partial_z = \{\partial_{z_i}\}_{i=1}^{2n}\). These are dual bases 
satisfying \(dz_i \partial_{z_j} = \delta_{ij}\). In the basis \(\{dz_i\}_{i=1}^{2n}\), the symplectic form \(\omega\) is 
given by

\[
\omega = \sum_{i,j}^{2n} \frac{1}{2} J_{ij} dz_j \wedge dz_i, \quad J_{ij} \in \mathbb{R}. \tag{9}
\]

The matrix \(J = [J_{ij}]\) satisfies \(J^2 = -I_{2n}\), and it is the representation of the 
complex structure associated to \(\omega\) in the basis \(\{dz_i\}_{i=1}^{2n}\). Remark that \(J\) is an 
antisymmetric matrix \(J + J^T = 0_{2n}\).

A Liouvillian form \(\theta\) on \((M, \omega)\) is expressed in the basis \(\{dz_i\}_{i=1}^{2n}\) by \(\theta = 
\sum_i \alpha_i(z) dz_i\), \(z = (z_1, z_2, \cdots, z_{2n}) \in M\), where \(\alpha_i : M \to \mathbb{R}\) are smooth functions 
of \(z\). Since

\[
\omega = d\theta = \sum_{i,j} \frac{\partial \alpha_j(z)}{\partial z_i} dz_i \wedge dz_j, \quad z = (z_1, z_2, \cdots, z_{2n}) \in M,
\]

and writing \(A(z) = [A_{ij}(z)] = \left[\frac{\partial \alpha_j(z)}{\partial z_i}\right]\) we have the decomposition in symmetric 
and antisymmetric components by

\[
A_s(z) = \frac{1}{2} (A(z) + A^T(z)) \quad \text{and} \quad A_a(z) = \frac{1}{2} (A(z) - A^T(z)).
\]
The condition for $\theta$ to be a Liouvillian form is $A_{\theta}(z) \equiv \frac{1}{2}J$, and denoting $A_{\theta}(z) = S(z)$ to remark it is a symmetric matrix, we have $A(z) = S(z) + \frac{1}{2}J$. Moreover, the symmetric part $S(z)$ belongs to the kernel of the differential $\theta \mapsto \omega$. We have proved the following:

**Lemma 5.1** The set of Liouvillian forms on an exact symplectic manifold $(M, \omega)$ is given in local coordinates by 1-forms $\theta = \sum_i \alpha_i(z)dz_i$ where the matrix $A(z) = \frac{\partial \alpha_i(z)}{\partial z_j}$ has the structure $A(z) = S(z) + \frac{1}{2}J$, where $S(z) = S^T(z)$ and $J$ is the complex structure associated to $\omega$ in the local coordinates $\{z_i\}_{i=1}^{2n}$.

Every exact symplectic manifold $(M, \omega)$ possesses a natural Liouvillian form $\theta_0$ given by the complex structure associated to the symplectic form $\omega$. The Liouvillian form $\theta_0$ has no symmetric component and we call it the elementary or basic Liouvillian form.

**Corollary 2** The elementary Liouvillian form in Darboux’s coordinates $z = (q, p) \in (M, \omega)$ is given by

$$\theta_0 = \frac{1}{2} \sum_{i=1}^{n} (p_i dq_i - q_i dp_i).$$  \hspace{1cm} (10)

Consider the tautological symplectomorphism $J$ as in Theorem 4.1.

**Lemma 5.2** The elementary Liouvillian form $\theta_0$ is invariant under the action of the complex structure, i.e. $\theta_0 = J^* \theta_0$.

Proof. Given local coordinates $z \in (M, \omega)$ the elementary Liouvillian form is given by $\theta_0 = \frac{1}{2} dz J z$. Consequently,

$$J^* \theta_0 = \frac{1}{2} (dz J^T) J (J z) = \frac{1}{2} dz J z = \theta_0.$$  \hspace{1cm} (11)

This lemma gives a Liouvillian form on an exact symplectic manifold, proving Theorem 4.1. The Liouvillian form $\theta = \pi_1^* \theta_0 - \pi_2^* \theta_0$ induces a natural symplectomorphism which will be associated to the mid-point rule. We will show this fact in the last section where we will construct numerical integrators from the symplectic maps coming from Liouvillian forms.

For studying the way a Liouvillian form induces a symplectic integrator we restrict our study to the set of Liouvillian forms with linear coefficients. It becomes a linear space over $\mathbb{R}$ with finite dimension. In the rest of this paper we replace the matrix $A(z)$ for a linear form $Az = (S + \frac{1}{2}J)z$ where $A$ and $S$ are constant matrices in $\mathbb{M}_{2n \times 2n}(\mathbb{R})$.

**Lemma 5.3** The space of Liouvillian forms with linear coefficients on a 2n-dimensional exact symplectic manifold $(M, \omega)$ has dimension $n(2n+1)$.

\hspace{1cm} \footnote{Remark that $dz$ is a covector and it transforms by the transpose $dz \mapsto dz J^T$.}
Proof. Applying Lemma 5.1 we deduce that the dimension of the space of Liouvillian forms is exactly the dimension of the space \( \text{Sym}(2n) \) of symmetric \( 2n \times 2n \) matrices \( S = S^T \), given by \( \dim \text{Sym}(2n) = \frac{1}{2}(2n)(2n + 1) = n(2n + 1) \). □

Remark 3 The space of Liouvillian forms with linear coefficients on a symplectic manifold \((M, \omega)\) is isomorphic to \( sp(M, \omega) \) as an affine space.

5.2 Liouvillian forms on the product manifold

We are interested on the space of Liouvillian forms with linear components on the product manifold \((\tilde{M}, \omega)\) given by

\[
\theta = \pi_1^* \theta_1 - \pi_2^* \theta_2, \quad \theta_i \in \Gamma(T^* M_i), \quad i = 1, 2,
\]

where \( \theta_i, i = 1, 2 \) are represented in local coordinates by \( \theta_i = dz_i (\frac{1}{2} J + S_i)z_i \), \( i = 1, 2 \) (see Lemma 5.1).

Lemma 5.4 Consider local coordinates \((z, Z) \in (\tilde{M}, \omega)\), where \( z \in M_1 \) and \( Z \in M_2 \). Liouvillian forms on \((\tilde{M}, \omega)\) given in (12) have a representation \( \theta = (dz, dZ) \tilde{A}(z, Z)^T \) for the matrix \( \tilde{A} = \tilde{S} + \frac{1}{2} \tilde{J} \), where \( \tilde{A} \in M_{4n \times 4n}(\mathbb{R}) \) is a symmetric matrix with the form

\[
\tilde{S} = \begin{pmatrix} S_1 & 0_{2n} \\ 0_{2n} & -S_2 \end{pmatrix}, \quad S_1, S_2, 0_{2n} \in M_{2n \times 2n}(\mathbb{R}), \quad S_i = S_i^T, \quad i = 1, 2.
\]

Proof. Consider a point on the product manifold \((z, Z)^T \in (\tilde{M}, \omega)\) written in local coordinates of the factors \( z \in M_1 \) and \( Z \in M_2 \). Using Lemma 5.1 \( \theta \) has a representation

\[
\theta = (dz, dZ) \tilde{A} \begin{pmatrix} z \\ Z \end{pmatrix}, \quad \tilde{A} = \tilde{S} + \frac{1}{2} \tilde{J},
\]

where \( \tilde{S} \) is a symmetric matrix of size \( 4n \times 4n \). The key property is the decomposition of the tangent bundle \( T\tilde{M} = TM_1 \oplus TM_2 \), since the representation of Liouvillian forms of type (12) is given by a matrix with two blocks

\[
\tilde{A} = \begin{pmatrix} \frac{1}{2} J + S_1 & 0_{2n} \\ 0_{2n} & -(\frac{1}{2} J + S_2) \end{pmatrix} = \begin{pmatrix} S_1 & 0_{2n} \\ 0_{2n} & -S_2 \end{pmatrix} + \frac{1}{2} \begin{pmatrix} J & 0_{2n} \\ 0_{2n} & -J \end{pmatrix} = \tilde{S} + \frac{1}{2} \tilde{J}
\]

proving the lemma. □

The (affine) space of Liouvillian forms with linear coefficients on \((\tilde{M}, \omega)\) has dimension \( \dim \text{Sym}(4n) = 2n(4n + 1) \) and the dimension of the subset of forms given by (12) is \( 2 \dim \text{Sym}(2n) = 2n(2n+1) \). However, just a subset of this space is adapted for the construction of numerical schemes. We will be interested in the particular case \( S = S_1 = -S_2 \) whose projection satisfies Condition 1. We will return to this argument when we study Hamiltonian systems in Section 8.
6 The implicit map from the projection of the Lagrangian submanifold

The linearization of \( \theta \) give us the local expresion of the vertical bundle \( V \Lambda \subset T \tilde{M} \) to the Lagrangian submanifold \( \Lambda \) and we want to recover the tangent bundle \( T \Lambda \subset T \tilde{M} \). Since the tangent bundle \( T \tilde{M} \) accepts a decomposition by \( T \tilde{M} = V \Lambda \oplus T \Lambda \) and the tangent bundle is mapped into the vertical bundle by \( V_z \Lambda = \tilde{J} T_z \Lambda \) for every \( z \in \Lambda \), then we recover locally the tangent spaces using the complex structure \( T_z \Lambda = \tilde{J} T_z (V_z \Lambda) \). We project this subbundle with the tangent projection \( TN = T\pi (T \Lambda) = T\pi (\tilde{J} T (V \Lambda)) \).

**Lemma 6.1** Let \((\tilde{M}, Q_1 \times Q_2, \theta, \pi, \Psi)\) be a special symplectic manifold and \( \Lambda \subset \tilde{M} \) be an integral submanifold for \( \theta = \pi_1^* \theta_1 - \pi_2^* \theta_2 \) where \( \theta_i = dz (\frac{1}{2} J + S_i) \). Then for every \( x \in \Lambda \), the subspaces \( T_{\pi_i(x)} \Lambda_i := T_{\pi_i} (\tilde{J} T (V_x \Lambda)) \subset T_x M_i, i = 1, 2 \) are Lagrangian with local expression \( L_i = (\frac{1}{2} I - JS_i)z \), satisfying \( (\frac{1}{2} J + S_i)z = 0 \), \( i = 1, 2 \).

**Proof.** Applying point 2) from Lemma 2.1, the projection of the Lagrangian submanifold \( \Lambda \in \tilde{M} \), by \( \pi_i(\Lambda) = \Lambda_i \subset M_i \) is a Lagrangian submanifold in \( M_i \), \( i = 1, 2 \). In local coordinates, the expressions

\[
L_i = (\frac{1}{2} I - JS_i)z \quad \text{and} \quad (\frac{1}{2} J + S_i)z = 0, \quad i = 1, 2,
\]

are the equations of the tangent space to the integral submanifold \( \Lambda_i \subset M_i \) defined by the Liouvillean form \( \theta_i = dz (\frac{1}{2} J + S_i) \). They define the same tangent space since \( \Lambda \) is an integral submanifold for \( \theta = \pi^* \theta_1 - \pi_2^* \theta_2 \) and \( \Lambda_i \) are integral submanifolds for \( \theta_i \).

We define the linear space given by the sum \( V = T_{\pi_1(x)} \Lambda_1 + T_{\pi_2(x)} \Lambda_2 \) as vector subspaces of \( T \tilde{M} \). Using Lemma 6.1 we can write \( V = L_1 + L_2 \). We want that \( V \) satisfies Condition 1, however, point 2) in Condition 1 is enough for a symplectic map as we will see below.

**Lemma 6.2** Define the implicit map induced by the sum of the linear spaces \( V = L_1 + L_2 \) from Lemma 6.1 given by

\[
\rho(z, Z) = (\frac{1}{2} I_{2n} - JS_1)z + (\frac{1}{2} I_{2n} + JS_2)Z.
\]

Then, \( \rho(z, z) = z \), if and only if \( S_1 = S_2 \).

**Proof.** Evaluating in \( (z, z) \in \Delta \subset \tilde{M} \) we have \( \rho(z, z) = z + J(S_2 - S_1)z \) which produces the identity on the diagonal, if and only if \( J(S_2 - S_1)z = 0 \).

---

5 The null space or the kernel of the projection \( T\pi \).
The implicit map induced by the projection of the lagrangian submanifold Λ adapted for the construction of symplectic maps is given in local coordinates of the product manifold \((z, Z) \in M\) by
\[
\rho(z, Z) = \frac{1}{2} (z + Z) + b(Z - z),
\]
where \(b \in M_{2n \times 2n}(\mathbb{R})\) is a Hamiltonian matrix.

7 The method of Liouvillian forms

The construction of implicit symplectic maps using the method of Liouvillian forms is obtained by restructuring the construction of the last section avoiding the explicit use of the special symplectic manifold. We recover all the information from two different (but related) Liouvillian forms and the complex structure.

1) For any exact symplectic manifold \((M, \omega)\) consider two copies \((M_i, \omega_i), i = 1, 2\) for the construction of the product manifold \((\tilde{M}, \omega_\ominus)\) and select a Liouvillian form \(\theta\) on \(\tilde{M}\).

We define the Liouvillian form satisfying Condition II in the following way: fix a Liouvillian form \(\theta_1\) with linear coefficients on \((M_1, \omega_1)\) and express it in local coordinates by \(\theta_1 = dz(\frac{1}{2}J + S)z\); define a second Liouvillian form on \((M_2, \omega_2)\) by \(\theta_2 = dZ(\frac{1}{2}J - S)Z\). The form
\[
\theta = \pi_1^* \theta_1 - \pi_2^* \theta_2,
\]
is Liouvillian on the product manifold. The expression of the vertical bundle in local coordinates is
\[
\begin{pmatrix} z \\ Z \end{pmatrix} \mapsto \begin{pmatrix} \frac{1}{2}J + S & 0_{2n} \\ 0_{2n} & -\frac{1}{2}J + S \end{pmatrix} \begin{pmatrix} z \\ Z \end{pmatrix}, \quad S \in M_{2n \times 2n}(\mathbb{R}), S = S^T.
\]

2) The Pfaffian equation \(\theta = 0\) defines implicitly and locally the Lagrangian submanifold \(\Lambda\). We use the complex structure \(\hat{J}\) associated to the symplectic form \(\omega_\ominus\) of the product manifold to obtain the equations of the tangent spaces by \(T\Lambda = \hat{J}TV\Lambda\). In local coordinates we have
\[
\begin{pmatrix} z \\ Z \end{pmatrix} \mapsto \begin{pmatrix} \frac{1}{2}I_{2n} - b & 0_{2n} \\ 0_{2n} & \frac{1}{2}I_{2n} + b \end{pmatrix} \begin{pmatrix} z \\ Z \end{pmatrix}, \quad b = JS \in M_{2n \times 2n}(\mathbb{R}), S = S^T.
\]

3) Project this Lagrangian subspace on the tangent bundle of the original symplectic manifold \(TM\) with \(T\pi_1(T\Lambda) + T\pi_2(T\Lambda)\) as linear subspaces. We will have the induced implicit map
\[
\rho(z, Z) = (\frac{1}{2}I_{2n} - b)z + (\frac{1}{2}I_{2n} + b)Z,
\]
where \(b \in M_{2n \times 2n}(\mathbb{R})\) is a Hamiltonian matrix.

4) Verify if
\[
TM = T\pi_1(T\Lambda) \oplus T\pi_2(T\Lambda) = T\Lambda_1 \oplus T\Lambda_2,
\]
which holds when the projected Lagrangian submanifolds are complementary. Since $z$ and $Z$ are two different close points, we only check if the implicit map restricted to the diagonal is the identity $\rho|_\Delta = I_{2n}$. The map (19) satisfies this condition by construction.

**Theorem 7.1** Let $(M,\omega)$ be an exact symplectic manifold of dimension $2n$ and $U \subset M$ a start-shaped open subset containing the points $z, Z \in U$. Define an implicit map $\rho : U \times U \to U$ by expression (19). The implicit map $(z, Z) \mapsto Z = \rho(z, Z)$ is symplectic.

**Proof.** We prove this result using implicit differentiation. Consider the implicit mapping $\Psi$ given by

$$\Psi(z, Z) = Z - \rho(z, Z) = 0.$$  (20)

Implicit differentiation of (20) gives

$$\frac{\partial \Psi(z, Z)}{\partial z} = -\frac{1}{2}I_{2n} + b \quad \text{and} \quad \frac{\partial \Psi(z, Z)}{\partial Z} = \frac{1}{2}I_{2n} - b.$$  (21)

Denoting the partial derivatives of $\Psi$ by

$$B_1 = -\frac{\partial \Psi(z, Z)}{\partial z} \quad \text{and} \quad B_2 = \frac{\partial \Psi(z, Z)}{\partial Z},$$

the amplification matrix of the linearized system (11) is given by $B = B_2^{-1} \circ B_1$, and $\Psi$ is symplectic if the matrix $B$ is symplectic. We use the fact that the transpose $B^T = B_1^T \circ B_2^{-T}$ of a symplectic matrix is symplectic to transform the symplecticity condition into $B_2^{-1} \circ B_1JB_1^T \circ B_2^{-T} = J$, or equivalently into $B_1JB_1^T - B_2JB_2^T = 0$. This condition is satisfied since $B_1 = B_2$, and the implicit map is symplectic as we want to prove. \qed

**Remark 4** The converse is in general not true since we are characterizing only symplectic maps solving a variational problem with particular boundary conditions.

We can consider the point $\bar{z} = \rho(z, Z)$ as an intermediate point on the path joining $z$ to $Z$ minimizing some variational problem. To develop this idea, we introduce some additional terminology. An implicit map $\phi : U \times U \to U$ is called consistent if there exist two explicit maps $\psi_1, \psi_2 : U \to U$ and a point $\bar{z} \in U$, such that

$$\bar{z} = \psi_1(z) \quad \text{and} \quad \bar{z} = \psi_2(Z).$$  (22)

We say that $\bar{z}$ is the point of consistency and $\psi = \psi_2^{-1} \circ \psi_1 : U \to U$ its consistency map. It is an explicit well defined map. We say that $\phi$ interleaves a symplectic map if its consistency map is symplectic.

We need a result from the Weyl’s extension of Cayley’s transformation. The interested readers are referred to [15] for the proof.
Lemma 7.2 (Generalized Cayley’s transformation) If the non-exceptional matrices $H$ and $S$ are connected by the relations

$$S = (I - H)(I + H)^{-1} = (I + H)^{-1}(I - H)$$
$$H = (I - S)(I + S)^{-1} = (I + S)^{-1}(I - S)$$

and $G$ is any matrix, then $S^TGS = G$ if and only if $H^TG + GH = 0$.

For the symplectic case, we fix the arbitrary matrix $G = J$ to the complex structure on $TM$. Now we can relate the induced implicit map $\rho$ with Cayley’s transformation in the following

Proposition 2 With the same hypotheses as Theorem 7.1, consider the explicit map $\psi = \psi_2^{-1} \circ \psi_1 : U \to U$ as the consistency map associated to the implicit map $\rho : TU \times TU \to TU$ given in (19). Then, the consistency map $\psi$ is symplectic and it corresponds to Cayley’s transformation of the matrix $2JS$.

Proof. Consider $\rho(z, Z)$ as a linear combination of two explicit linear maps coming from $z$ and $Z$, in the form $\rho(z, Z) = \frac{1}{2}(T\psi_1(z) + T\psi_2(Z))$. From expression (19), we can write explicitly

$$T\psi_1(z) = (I_{2n} - 2JS)z \quad \text{and} \quad T\psi_2(Z) = (I_{2n} + 2JS)Z. \quad (23)$$

Since $S \in M_{2n \times 2n}(\mathbb{R})$ is a symmetric matrix, the matrix $H = 2JS$ is Hamiltonian. In this case, the consistency map associated to $\rho(z, Z)$ is given by

$$\psi = \psi_2^{-1} \circ \psi_1,$$

whose linearization gives

$$T\psi = T\psi_2^{-1} \circ T\psi_1 = (I_{2n} + H)^{-1}(I_{2n} - H). \quad (24)$$

This is the symplectic Cayley’s transformation of the Hamiltonian matrix $H$. Applying Weyl’s Lemma we obtain immediately that the consistency map $\psi : U \ni z \mapsto Z = \psi(z) \in U$ is symplectic. □

Corollary 3 For every symplectic mapping $\psi \in Sp(M, \omega)$ on an exact symplectic manifold, there exists a Liouvillian form $\theta_\psi$ adapted to $\psi$.

Proof. Suppose $\psi \in Sp(M, \omega)$ is represented at every point $m \in M$ by a non-exceptional matrix $S \in Sp(2n)$. There exists an associated Hamiltonian matrix given by the symplectic Cayley’s transformation $H = (I_{2n} - S)(I_{2n} + S)^{-1}$. Consequently, the linearization of the Liouvillian form $\theta_\psi$ adapted to $\psi$ is given by some square matrix $R = \frac{1}{2}J(I_{2n} + H)$ in the form $\theta_\psi = dzRz$. Moreover, the implicit map $\rho : TU \times TU \to TU$ in coordinates $(z, Z) \in U \times U$ is defined in terms of $H$ by

$$\rho(z, Z) = \left(\frac{1}{2}I_{2n} - \frac{1}{2}H\right)z + \left(\frac{1}{2}I_{2n} + \frac{1}{2}H\right)Z. \quad (25)$$

- A matrix $A \in GL(n)$ is said to be non-exceptional if $\det(I + A) \neq 0$, where $I$ is the identity matrix in $GL(n)$. 

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Consider the matrix $G$ in Weyl’s lemma as a bilinear form $u^T G v$. The trivial case $G = I_{2n}$ gives the Euclidean metric and the Cayley’s transformation relates symmetric with antisymmetric matrices. The case $G = J$ is the symplectic form and it relates symplectic with Hamiltonian matrices. In [6] we show that this property with an additional dependency on a parameter discretizing time produce reversible maps.

8 Hamiltonian systems and implicit symplectic integrators

The numerical simulation of Hamiltonian vector fields is made by numerical schemes called symplectic algorithms or symplectic integrators. We introduce the notation and terminology for the application of Liouvillian forms in symplectic integration.

A Hamiltonian system $(M, \omega, X_H)$ is a vector field $X = X_H$ on a symplectic manifold $(M, \omega)$ such that inner product of the symplectic form and the vector field satisfies $i_{X_H} \omega = -dH$, for a differentiable function $H : M \to \mathbb{R}$.

The set of solutions $\varphi^t_H : M \times \mathbb{R} \to M$ of the Hamiltonian vector field $X_H$ is called the flow of $X_H$ and it is defined by

$$\frac{d}{dt} \varphi^t_H(z) = X_H(\varphi^t_H(z)).$$

(26)

The flow is a 1-parameter subgroup of symplectic diffeomorphisms with parameter $t \in \mathbb{R}$. For every point $z_0 \in M$, the solution $\varphi^t_H(z_0)$ is the integral curve of $X_H$ passing by $z_0$ at time $t = 0$.

A symplectic algorithm with stepsize $h$, is the numerical approximation $\psi_h$ of the map $\varphi^h_H$, for $t = h$ fixed, which is smooth with respect to $h$ and $H$, and preserves the symplectic form $(\psi_h)^* \omega = \omega$. Consider an open set $U \subset M$ and two points on the flow of $X_H$, say $z_t = \varphi^t(z_0)$ and $z_{t+h} = \varphi^{t+h}_H(z_0)$. By the group property of the flow, it is enough to perform the analysis around $t = 0$, then the points will be denoted by $z_0$ and $z_h$.

**Theorem 8.1** Let $(M, \theta, X_H)$ be a Hamiltonian system on an exact symplectic manifold. Consider a convex open set $U \subset M$ containing the points $z_0$ and $z_h$ on the flow of $X_H$. If an implicit map $\rho : U \times U \to U$ is defined by

$$\rho(z_0, z_h) = \left( \frac{1}{2} I_{2n} - b \right) z_0 + \left( \frac{1}{2} I_{2n} + b \right) z_h,$$

(27)

where $b$ is a Hamiltonian matrix in $M_{2n \times 2n}(\mathbb{R})$, then, the map

$$z_h = z_0 + h X_H \circ \rho(z_0, z_h)$$

is symplectic.
Proof. Since $X_H$ is a Hamiltonian vector field, invariant under symplectic transformations, it suffices that $\rho(z_0, z_h)$ be a symplectic map. Applying Theorem 7.1 we obtain the desired result. □

An alternative proof of the theorem is using implicit differentiation. Consider the implicit mapping $\Psi$ given by

$$
\Psi(z_0, z_h) = z_h - z_0 - hX_H \circ \rho(z_0, z_h) = 0 \quad (28)
$$

as in the proof of Theorem 7.1. Implicit differentiation of (28) using the chain rule gives

$$
B_1 := \frac{\partial \Psi(z_0, z_h)}{\partial z_0} = I_{2n} - hH \left( \frac{1}{2} I_{2n} - b \right) \quad (29)
$$

$$
B_2 := \frac{\partial \Psi(z_0, z_h)}{\partial z_h} = -I_{2n} - hH \left( \frac{1}{2} I_{2n} + b \right) \quad (30)
$$

where $H$ is a Hamiltonian matrix given by $H = JD^2H$ and $D^2H$ is the Hessian matrix of $H$. The symplecticity test $B_1JB_1^T - B_2JB_2^T = 0$ is satisfied since $H$ and $b$ are Hamiltonian matrices.

8.1 The generalized implicit symplectic Euler scheme

The relevance of this method is that we have a linear (continuous) space of dimension $n(2n+1)$ where we can select Hamiltonian matrices for the construction of numerical schemes. Using Theorem 8.1 we are able to define the generalized implicit symplectic Euler scheme as the map given by

$$
\psi_h : U \times U \to U
$$

$$
(z_0, z_h) \mapsto z_h = z_0 + hX_H(\bar{z}) \quad (31)
$$

where $\bar{z} = \frac{1}{2}(z_0 + z_h) + b(z_h - z_0)$ and it corresponds to the map $\bar{z} = \rho(z_0, z_h)$ given by the expression (27).

Remark 5 In a slightly different context, Feng Kang (unpublished) has shown that generating functions obtained by some particular type of matrices $\alpha \in M_{4n \times 4n}(\mathbb{R})$ can be reduced to generating functions constructed by an equivalent simplified matrix containing the two submatrices given in expression (27) (see Ge and Dau-lui [3]). In their method, those matrices are the input for the evolutive Hamilton-Jacobi equation.

Proposition 3 The elementary Liouvillean form $\theta_0$ on an exact symplectic manifold $(M, \omega)$, produces a Liouvillean form on the product manifold $(\bar{M}, \omega_\otimes)$ given by $\theta = \pi_1^*\theta_0 - \pi_2^*\theta_0 = \frac{1}{2}dz_0Jz_0 - \frac{1}{2}dz_hJz_h$. In Darboux’s coordinates it corresponds to

$$
\theta = \frac{1}{2} (p_0 dq_0 - q_0 dp_0 - p_h dq_h + q_h dp_h), \quad (32)
$$

whose generalized symplectic Euler scheme is the symplectic mid-point rule.
Proof. It is a direct computation using the fact that elementary Liouvillian form does not have a symmetric component. In terms of the generalized symplectic Euler scheme, their argument $\bar{z}$ have a null Hamiltonian matrix $b = 0_{2n}$. The argument $\bar{z} = \frac{1}{2}(z_0 + z_h)$ gives the scheme
\[ z_h = z_0 + hX_H \left( \frac{1}{2}(z_0 + z_h) \right), \]
which is the mid-point rule. □

Proposition 4 In terms of the generalized symplectic Euler scheme (31) with Darboux’s coordinates $z_0 = (q_0, p_0)^T$ and $z_h = (q_h, p_h)^T$, the Hamiltonian matrices
\[ b_A = \frac{1}{2} \begin{pmatrix} -I & 0 \\ 0 & I \end{pmatrix}, \quad b_B = \frac{1}{2} \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \quad b \in M_{2n \times 2n}(\mathbb{R}). \]
corresponds to the symplectic Euler $A$ and $B$ schemes, respectively.

Proof. Write the sum and difference vectors in Darboux’s coordinates by
\[ \frac{1}{2}(z_0 + z_h) = \frac{1}{2} \begin{pmatrix} q_0 + q_h \\ p_0 + p_h \end{pmatrix}, \quad \text{and} \quad (z_h - z_0) = \begin{pmatrix} q_h - q_0 \\ p_h - p_0 \end{pmatrix}. \]
Computing $b_A(z_h - z_0)$ leads to $b_A(z_h - z_0) = \frac{1}{2} (q_0 - q_h, p_h - p_0)^T$ and consequently $\bar{z} = \frac{1}{2}(z_0 + z_h) + b_A(z_h - z_0)$ produces $\bar{z} = (q_0, p_0)^T$. In the same way $\bar{z} = \frac{1}{2}(z_0 + z_h) + b_B(z_h - z_0)$ produces $\bar{z} = (q_h, p_0)^T$. Using these arguments in the generalized scheme (31) we obtain the standard Euler schemes. □

9 Two families of implicit symplectic integrators

In this section we develop two examples of the application of the method of Liouvillian forms for constructing symplectic integrators. The first one considers the construction of the special symplectic manifold on $Q_1 \times Q_2$, using the symplectomorphism $\Psi : \tilde{M} \rightarrow T^*(Q_1 \times Q_2)$. The second one is given for applying the method directly. In the practice, we will use the generalized symplectic Euler scheme given in (31).

9.1 Example 1: A simple family from symplectic rotations

Here, we explicitly define the symplectomorphism between the product manifold $(\tilde{M}, \omega_{\otimes})$ and the cotangent bundle $T^*(Q_1 \times Q_2)$ using a family of symplectic rotations. We take the loop of symplectic rotations induced by the complex structure $J \mapsto \exp(\varphi J)$ on the product manifold $(\tilde{M}, \omega_{\otimes})$.

Lemma 9.1 If $\tilde{J}$ is a complex structure then $\exp(\varphi \tilde{J}) = \cos(\varphi)I_{4n} + \sin(\varphi)\tilde{J}$. 

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Proof. Use $\tilde{J}^2 = -I_{4n}$ in the development of the exponential. Define the symplectic rotation $R_\phi \in \text{Sp}(\tilde{M}, \omega_\otimes)$ by $R_\phi = \exp(\phi J)$ and define the curve of diffeomorphisms $\Psi_\phi = E_1 \circ R_\phi$, $\phi \in [0, \pi/2]$.

Given symplectic coordinates $(q_0, p_0, q_h, p_h) \in \tilde{M}$ and $(x_0, x_h, y_0, y_h) \in T^*(Q_1 \times Q_2)$, the diffeomorphism $\Psi_\phi : \tilde{M} \to T^*(Q_1 \times Q_2)$ pulls-back the Liouville form $\theta_{Q_1 \times Q_2} = y_0 dx_0 + y_h dx_h$ into $\theta_\phi = \Psi_\phi^* \theta_{Q_1 \times Q_2}$ expressed in these coordinates by

$$
\theta_\phi = \cos^2 \phi p_0 dq_0 - \sin^2 \phi p_h dq_h - \sin^2 \phi q_0 dp_0 + \cos^2 \phi q_h dp_h + \cos \phi \sin \phi (q_0 dq_0 - p_0 dp_0) + \cos \phi \sin \phi (q_h dq_h - p_h dp_h)
$$

(34)

The quintuple $\left(\tilde{M}, (Q_1 \times Q_2), \theta_\phi, \pi, \Psi_\phi\right)$ is a family of special symplectic manifolds on $Q_1 \times Q_2$. We have the following

**Lemma 9.2** The set of forms (34) is a 1-parameter family of Liouvillian forms. The path $\theta_\phi$ contains the Liouvillian forms associated to the generating functions of type II and type III.

Proof. By a direct computation we obtain $d\theta_\phi = dp_0 \wedge dq_0 - dp_h \wedge dq_h = \omega_\otimes$, showing that any element in the family is Liouvillian on $(\tilde{M}, \omega_\otimes)$. The forms at the values $\phi = 0$ and $\phi = \pi/2$ are

$$
\theta_\phi|_{\phi=0} = p_0 dq_0 + q_h dp_h \quad \text{and} \quad \theta_\phi|_{\phi=\pi/2} = -q_0 dp_0 - p_h dq_h.
$$

By Lemma 4.2 they are associated to generating functions of type II and III, respectively. □

The family of vertical fibers to $\Lambda_\phi \subset \tilde{M}$, associated to the Liouvillian forms $\theta_\phi$ is given by equations

$$
\begin{align*}
\dot{q}_0 &= \cos^2 \phi p_0 + \cos \phi \sin \phi q_0, & \dot{p}_0 &= -\sin^2 \phi q_0 - \cos \phi \sin \phi p_0, \\
\dot{q}_h &= -\sin^2 \phi p_h + \cos \phi \sin \phi q_h, & \dot{p}_h &= \cos^2 \phi q_h - \cos \phi \sin \phi p_h.
\end{align*}
$$

We obtain the tangent fibers by left multiplying vertical fibers by $\tilde{J}^T$, mapping $(\dot{q}_0, \dot{p}_0, \dot{q}_h, \dot{p}_h) \mapsto (-\dot{p}_0, \dot{q}_0, \dot{p}_h, -\dot{q}_h)$. Finally, the projection $T\pi(T\Lambda_\phi) \cong T\pi_1(T\Lambda_\phi) \oplus T\pi_2(T\Lambda_\phi)$ in local coordinates is $\rho(q_0, p_0, q_h, p_h) = (\dot{p}_h - \dot{p}_0, \dot{q}_0 - \dot{q}_h)$, or explicitly by

$$
\begin{align*}
\dot{q}_h &= \cos^2 \phi q_h + \sin^2 \phi q_0 + \cos \phi \sin \phi (p_0 - p_h) \\
\dot{p}_h &= \cos^2 \phi p_h + \sin^2 \phi q_h + \cos \phi \sin \phi (q_0 - q_h).
\end{align*}
$$

(35)

The family of implicit symplectic integrators is given by

$$
q_h = q_0 + h \frac{\partial \rho}{\partial q} (\bar{q}_0, \bar{p}_0) \\
p_h = p_0 - h \frac{\partial \rho}{\partial p} (\bar{q}_0, \bar{p}_0).
$$

(36)

Evaluating these coordinates in $\phi = 0$ and $\phi = \pi/2$ we obtain

$$
(\bar{q}_0, \bar{p}_0)|_{\phi=0} = (q_0, p_0) \quad \text{and} \quad (\bar{q}_0, \bar{p}_0)|_{\phi=\pi/2} = (q_0, p_h).
$$

(37)

We have proved the following result.
Corollary 4 The implicit scheme \( z_h = z_0 + hX_H \circ \rho(z_0, z_h) \) where the linear map \( \rho(z_0, z_h) = (\bar{q}_h, \bar{p}_h) \) is defined by the expression (35), is a family of symplectic integrators which joins the symplectic Euler schemes A and B.

Using the identities

\[
\cos \phi \sin \phi = \frac{\sin 2\phi}{2}, \quad \sin^2 \phi = \frac{1 - \cos 2\phi}{2}, \quad \cos^2 \phi = \frac{1 + \cos 2\phi}{2},
\]

we rewrite (35) in compact form \( \bar{z} = (\bar{q}_h, \bar{p}_h) \) by \( \bar{z} = \frac{1}{2}(z_0 + z_h) + b(z_h - z_0), \) where

\[
b = \frac{1}{2} \begin{pmatrix}
-\cos 2\phi & \sin 2\phi \\
\sin 2\phi & \cos 2\phi
\end{pmatrix}, \quad b \in M_{2n \times 2n}(\mathbb{R}). \tag{38}
\]

9.2 Example 2: A three-parameter family

The method of Liouvillian forms applied to the construction of symplectic integrators yields the generalized symplectic Euler scheme (31). This scheme uses the argument \( \bar{z} = \frac{1}{2}(z_0 + z_h) + b(z_h - z_0), \) where \( b \in M_{2 \times 2}(\mathbb{R}) \) is an arbitrary Hamiltonian matrix. In a problem with 1 degree of freedom, \( b \) is a matrix of the form

\[
b = \begin{pmatrix}
\alpha & \beta \\
\gamma & -\alpha
\end{pmatrix}, \quad \alpha, \beta, \gamma \in \mathbb{R}.
\]

These are three free parameters in the generalized Euler method. Explicitly we have the numerical scheme

\[
q_h = q_0 + h \frac{\partial H}{\partial \bar{q}} (\bar{q}, \bar{p}) \quad \text{and} \quad p_h = p_0 - h \frac{\partial H}{\partial \bar{p}} (\bar{q}, \bar{p}), \tag{39}
\]

where

\[
\bar{q} = \frac{1}{2} - \alpha \right) q_0 + \left( \frac{1}{2} + \alpha \right) q_h + \beta (p_h - p_0)
\]

\[
\bar{p} = \left( \frac{1}{2} + \alpha \right) q_0 + \left( \frac{1}{2} - \alpha \right) q_h + \gamma (q_h - q_0),
\]

and \( \alpha, \beta, \gamma < h^2 < \frac{1}{4} \) have small values. Parameter \( \alpha \) modifies the symmetry of the oscillations with respect to time and the limiting cases \( (\alpha, \beta, \gamma) = (-\frac{1}{2}, 0, 0) \) and \( (\alpha, \beta, \gamma) = (\frac{1}{2}, 0, 0) \) are the usual symplectic Euler A and B integrators.

The parameters \( \{\alpha, \beta, \gamma\} \) modify the error and the oscillations of the numerical integrator around the orbits of the Hamiltonian flow. This fact has a geometrical justification that we develop in [5]. In a parallel article [6], we make a numerical study of this family explaining the oscillations of the numerical solution around the exact solution using a variational point of view.

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