An algorithm to generate canonical transformations: application to normal forms.

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Abstract

We describe a new method to generate symplectic diffeomorphisms. This method is based on primitive functions, and it was introduced in [24]. We apply the algorithm to the construction of normal forms of KAM tori. A concrete application, developed in detail and implemented numerically, is normal forms near invariant circles.

Keywords: Canonical transformations, KAM tori, normal forms, symplectic geometry.

1 Introduction

There are two classical ways to construct symplectomorphisms (the canonical transformations of mechanics): using generating functions and using Lie series. In [24] we proposed a new one, involving the so called *primitive function*.

The new method shares some qualities of the generating function method and the Lie series method. The primitive function generates the transformation, but one can work out the construction without involving mixed variables, and therefore inversion problems are eliminated. This combination makes the new algorithm more appropriate for numerical work. Moreover, the new algorithm does not have some of the restrictions of the classical ones, namely, it can be applied to degenerate cases.

The goal of this paper is to discuss the numerical analysis issues of the new algorithm and, much more important, to use this algorithm as a tool to study dynamical systems. In particular, we construct normal forms of KAM tori. As a numerical application, we present the implementation of the computation of the normal form of a KAM torus for an area preserving map.

As it is well known, normal forms are used in dynamical systems to classify invariant objects (fixed points, periodic orbits, invariant tori, etc.), to obtain information about the dynamics around the invariant object and to analyse bifurcations in parameter depending dynamical systems (see, for instance, [4, 9]). In Hamiltonian/symplectic dynamics, the normalizing transformations that reduce the Hamiltonian/symplectomorphism to a simpler form are canonical.

Therefore, the methods developed in this paper are a tool to classify a KAM torus by the coefficients of its normal form, to obtain information about the dynamics in its proximity, and to analyse bifurcations of KAM tori. Since the algorithm can be applied to degenerate cases, it helps to study shearless tori [11] and study bifurcations. Another application is the construction of approximate first integrals in a neighbourhood of the invariant surface [37].

In fact, canonical transformations are widely used in many branches of mathematics and physics (dynamical systems, celestial mechanics, optics, fluid mechanics, quantum mechanics, etc.), and there exists a very extensive literature on this subject.

For instance, the use of canonical transformations to obtain formal integrals of an autonomous Hamiltonian system (near an elliptic equilibrium point) goes back to Birkhoff [6], and he used generating functions (see also [22]). Hori [25] and Deprit [16] developed a formal theory of transforming the equations of motion in celestial mechanics based on Lie series. KAM Theory, founded by Kolgomorov [27], Arnold [2] and Moser [31], and the very related study of the diffusion in Hamiltonian systems (known as Arnold's diffusion [3]) and Nekhorosehv's theory [32, 19] are also indebted to the methods of canonical transformations theory. Bryuno has written some surveys on normal forms for Hamiltonian systems [7, 8]. Numerical applications of the normal form methodology in Hamiltonian systems (mainly in celestial mechanics) have been also developed by Simó [35], Jorba [26] and coworkers. Non-twist maps and shearless tori appear in plasma physics (see, for instance, Morrison's paper [30]) and fluid mechanics [10]. The list of references if very far from being complete, as well as the amount of applications and examples.

2 Preliminaries

Since in this paper we are interested in numerical applications, instead of considering a general phase space, we are going to focus from the very beginning on $\mathbb{T}^d \times \mathbb{R}^d$, where $\mathbb{T}^d = \mathbb{R}^d/\mathbb{Z}^d$. In fact, this example appears very often in the literature, for instance, in KAM theory. The general theory works in many exact symplectic manifolds [24]. Since in numerical implementations we need expansions, we have to adapt the general theory to this case.

Let $\mathbb{T}^d \times \mathbb{R}^d$ be the phase space, and denote by $(x,y) = (x_1,\dots,x_d,y_1,\dots,y_d)$ the angle-action coordinates. The *canonical symplectic form*

$$\omega = \mathrm{d}y \wedge \mathrm{d}x = \sum_{i=1}^{d} \mathrm{d}y_i \wedge \mathrm{d}x_i$$

has the extra feature of being exact. That is, there exist a 1-form α (an *action form*), such that $\omega = \mathrm{d}\alpha$. From here, the action form is the *Liouville* form on $\mathbb{T}^d \times \mathbb{R}^d \simeq T^*\mathbb{T}^d$:

$$\alpha = y\ \mathrm{d}x = \sum_{i=1}^{d} y_i\ \mathrm{d}x_i\ .$$

Let $F : \mathbb{T}^d \times \mathbb{R}^d \to \mathbb{T}^d \times \mathbb{R}^d$ be a diffeomorphism given by

$$\bar{x} = x + f(x,y) \pmod 1 \ , \ \bar{y} = g(x,y) \ , \tag{1}$$

where f and g are 1-periodic in the x variables.

F is a symplectomorphism if $F^*\omega = \omega$. This means that the 1-form $F^*\alpha - \alpha$ is closed. If this 1-form is not only closed, but also exact, that is, there exists a function $S : \mathbb{T}^d \times \mathbb{R}^d \to \mathbb{R}$ such that $F^*\alpha - \alpha = \mathrm{d}S$, we say that F is an *exact symplectomorphism* and that S is a *primitive function.* Writing this equation in coordinates it reads

$$\frac{\partial S}{\partial x} = \bar{y}^\top \frac{\partial \bar{x}}{\partial x} - y^\top \quad , \quad \frac{\partial S}{\partial y} = \bar{y}^\top \frac{\partial \bar{x}}{\partial y} \ . \tag{2}$$

Notice that the choice of the action form α (and, hence, of the geometry of phase space) leads to the choice of the primitive function.

Generating functions customary in mechanics (see e.g. [5]) and primitive functions are closely related [24]. The main difference is that a function S such that $F^*\alpha - \alpha = \mathrm{d}S$ does not produces an unique F, but a family of exact symplectomorphisms. The reason is the existence of a family of exact symplectomorphisms L for which $L^*\alpha = \alpha$ (for our election of α, the symplectic *lifts* of diffeomorphisms on $\mathbb{T}^d$, also known in mechanics as *point transformations*). So, we cannot expect full determination from S.

A special class of exact symplectomorphisms are those that fix all the points of the zero-section $\mathbb{T}^d \times \{0\}$. In [24], we constructed such an exact symplectomorphism from its primitive function. So, since an exact symplectomorphism that fixes all the points of $\mathbb{T}^d \times \{0\}$ is completely determined by its primitive function we are going to refer to it as a *primitive symplectomorphism.*

Recall that the twist of F at the point (x, y) is the matrix $\frac{\partial \bar{x}}{\partial y}(x, y)$. We say that F is a twist symplectomorphism if this matrix is non-degenerate at all. In this case, it is possible to construct (locally) a Lagrangian generating function (the generating function involving x and $\bar{x}$ coordinates). Notice that we do not need extra conditions on derivatives to construct F from its primitive function. So then, we can construct twist and non-twist dynamics by using the primitive function methods.

Next section is a review of the algorithm to compute a primitive symplectomorphism from its primitive function [24]. We complete the explanation in Appendix A. We compare the algorithm with some classical algorithms (using generating functions and Lie series) in Appendix B.

Section 4 is devoted to the algorithm for the computation of normal forms of KAM tori. The normal form transformation is the map that we have called a TLP symplectomorphism: a composition of a primitive symplectomorphism, a lift and a vertical translation. This combination of different dynamical behaviours makes TLP symplectomorphisms useful to codify symplectomorphisms.

Section 5 is a report of some numerical experiments. The implementations in a computer have been made in the case $d = 1$. This is the lower dimensional case, which is a natural first step. Firstly, we produce TLP symplectomorphisms, showing different types of dynamics. Secondly, we compute normal forms of rotational invariant curves in area preserving maps. Two models have been considered, both of them appear very often in the literature: the standard map and the quadratic standard map. Notice that the first one is a twist map, while the second one is not.

In spite of the fact that there are many methods in the literature to compute KAM tori (see, for instance, [28]), for the sake of completeness we explain an algorithm in Appendix C. Finally, a digression on primitive functions and algorithms to generate exact symplectomorphisms is included in Appendix D.

3 The primitive function algorithm

In [24], an algorithm to generate a primitive symplectomorphism from its primitive function was proposed. Recall that an exact symplectomorphism F given by (1), whose primitive function S satisfies (2), fix the zero-section $\{y = 0\}$ if an only if $\mathrm{D}S(x, 0) = 0$ for all the points on the zero-section. Recall also that primitive symplectomorphisms non only fix the zero-section, but also fix the points on the zero-section: $f(x, 0) = 0$ and $g(x, 0) = 0$.

The algorithm is based on the next construction. From (2), we obtain the equations

$$\begin{array}{rcl} f(x,y) & = & \mathbf{L}_y^{-1}\left(\nabla_y S - (\mathrm{D}_y f)^\top (g-y)\right)(x,y) \ , \\ g(x,y) & = & y + \nabla_x S(x,y) - (\mathrm{D}_x f(x,y))^\top g(x,y) \ , \end{array} \tag{3}$$

where $\mathbf{L}_y$ is the linear differential operator that acts on maps $h : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d$ such that $h(x, 0) = 0$, and it is defined by

$$\mathbf{L}_y h(x,y) = (\mathrm{D}_y h(x,y))^\top y \ .$$

This operator is studied in Appendix A. As a result

$$\mathbf{L}_y^{-1} H(x,y) = -H(x,y) + \int_0^1 \mathrm{D}_y H(x,ty)^\top y \ dt + \int_0^1 \frac{1}{t} H(x,ty)^\top y \ dt \ .$$

Notice that if H is a homogeneous vector function in the y variables, then $\mathbf{L}_y^{-1}(H)$ is also homogeneous of the same degree. This property lets us to obtain the recurrences of the next theorem, which was proven in [24].

Theorem 1 *Let $S : \mathbb{T}^d \times \mathbb{R}^d \to \mathbb{R}$ be an analytic function given by the convergent Fourier-Taylor series*

$$S(x,y) \ = \ \sum_{|n|\geq 2} S_n(x) y^n \ .$$

There is one and only one primitive symplectomorphism $F : \mathbb{T}^d \times \mathbb{R}^d \to \mathbb{T}^d \times \mathbb{R}^d$ whose primitive function is S. Moreover, F can be expanded in a neighbourhood of the zero-section as the convergent series

$$\bar{x} = x + \sum_{|n|\geq 1} f_n(x) y^n \ , \ \bar{y} = \sum_{|n|\geq 1} g_n(x) y^n \ ,$$

where the coefficients $f_n = (f_n^1, \dots, f_n^d)$ and $g_n = (g_n^1, \dots, g_n^d)$ satisfy the following recurrence relations:

$$k = 1: \qquad g_{e_i}^j = \delta_{ij} \ , \ f_{e_i}^j = (1+\delta_{ij}) \ S_{e_i+e_j} \quad (i, j = 1, \dots d) \ ;$$

$$k > 1: \qquad g_n^j = \frac{\partial S_n}{\partial x_j}(x) - \sum_i \sum_{\substack{u+v=n \\ u \neq 0, n}} \frac{\partial f_u^i}{\partial x_j}(x) g_v^i(x) \ ,$$

$$f_n^j = \frac{n_j + 1}{k} \left(S_{n+e_j}(x) + \sum_l F_{n+e_j-e_l}^l(x) \right) - F_n^j(x) \ ,$$

where $|n| = k, j \in \{1, \dots d\}$ and

$$F_n^j(x) = -\sum_i \sum_{\substack{u+v=n \\ |v| > 1}} (u_j + 1) f_{u+e_j}^i(x) g_v^i(x).$$

So, the expansions for F converge in a neighbourhood of the zero-section if S is analytic. Notice that if we are given S to order N, that is, $S_{\leq N}(x, y) = \sum_{2\leq|n|\leq N} S_n(x) y^n$, we can compute $f_{<N}$ and $g_{\leq N}$ (with the obvious notation). Notice also that if S is non analytical, but C^r or C^∞, the previous construction let us to obtain the jets (Fourier-Taylor expansions) of f and g from the jet of S. That is to say, the expansions for F are asymptotic if S is asymptotic.

We can read Theorem 1 as an algorithm, where the input is a Fourier-Taylor expansion S (up to a certain order), and the output is given by the corresponding jets of f and g. Notice that neither composition operators nor inversion problems appear in the algorithm. In the case $d = 1$, the algorithm reads as follows.

Algorithm 1 *Let $S : \mathbb{T} \times \mathbb{R} \to \mathbb{R}$ be a function whose Fourier-Taylor expansion is*

$$S(x, y) = \sum_{n\geq 2} S_n(x) y^n \quad \text{(input)}.$$

The only primitive symplectomorphism F whose primitive function is S can be expanded by

$$\bar{x} = x + \sum_{n\geq 1} f_n(x) y^n \ , \ \bar{y} = \sum_{n\geq 1} g_n(x) y^n \quad \text{(output)},$$

where the coefficients $f_n(x)$ and $g_n(x)$ are computed by the recurrence

$$\begin{aligned}
&\textit{step 1:} && g_1(x) = 1 \ ; \\
&\textit{step n:} && f_{n-1}(x) = \frac{n}{n-1} S_n(x) - \frac{1}{n-1} \sum_{u=1}^{n-2} u f_u(x) g_{n-u}(x) \ , \\
& && g_n(x) = S_n'(x) - f_{n-1}'(x) - \sum_{u=1}^{n-2} f_u'(x) g_{n-u}(x) \ .
\end{aligned}$$

Hence, if we are given $S_{\leq N}(x,y)$, we can compute $f_{<N}$ and $g_{\leq N}$.

Some technical issues of the algorithm. In order to implement the calculation on a computer, we have to write a set of procedures to manage Fourier series. The initial data –the function S– is a Taylor series in the y variables whose coefficients are Fourier series in the x variables. Of course, since the computer memory is finite, we have to cut off the Taylor series to a certain order N, and also its Fourier coefficients. We compute the coefficients f_n and g_n, which expand F iteratively, to order N (that is, the last coefficients that are computed are f_{N-1} and g_N). Besides round off errors and cut off errors, the coefficients are computed exactly, and we just need to add, to multiply and to differentiate Fourier series.

Once we have computed the expansions f and g, we can evaluate them at any point (x,y), by evaluating firstly their coefficients $f_n(x)$ and $g_n(x)$ and then applying Horner's rule. We recover the dynamics (the orbits) by iterating F.

Number of Fourier products. From the computational point of view, the most expensive operation is the product of Fourier series (the coefficients of the Taylor series). As in the step n we do $2n-4$ products, if we want to compute the expansions to order N in y, we have to do N^2-3N+2 products. In summary, the number of products of Fourier series needed to reach order N in the expansions is $O(N^2)$. In Appendix B we compare this cost with the corresponding costs when using the classical methods.

4 Normal forms of KAM tori

In this section we present an algorithm to compute the normal form around a KAM torus (cf. [24]).

For our purposes, a KAM torus of an exact symplectomorphism $F : \mathbb{T}^d \times \mathbb{R}^d \to \mathbb{T}^d \times \mathbb{R}^d$ is an invariant torus that is a Lagrangian graph

$$y = \nabla_x L(x) \ , \tag{4}$$

where the *generating function* of the graph $L(x) = a \cdot x + l(x)$ is given by the average $a \in \mathbb{R}^d$ and the periodic function $l : \mathbb{T}^d \to \mathbb{R}$, and the dynamics on the torus is conjugated to a rotation by $\omega \in \mathbb{T}^d$. This means that the invariance condition

$$\nabla_x L(\bar{x}(x, \nabla_x L(x))) = \bar{y}(x, \nabla_x L(x)) \tag{5}$$

is satisfied and that there exists a conjugation $\phi : \mathbb{T}^d \to \mathbb{T}^d$ given by

$$x = \theta + \varphi(\theta) \pmod 1 ,$$

where φ is 1-periodic in θ, such that

$$\bar{x}(\phi(\theta), \nabla_x L(\phi(\theta))) = \phi(\theta + \omega) . \tag{6}$$

There are several methods to construct KAM tori. Lindstedt method uses expansions of the torus with respect to the parameters that introduce non integrability in the system [17] . A method based on the Lagrangian formalism is useful when twist properties are satisfied, and the algorithm has been even implemented as computer assisted proofs [33]. Recently, the existence of Lagrangian tori in degenerate situations has been proved [14], and tori that are not graphs have been produced [20]. Since the list of previous references is far from being complete, the reader can obtain many information about these methods, and also about general results on KAM theory, from [28]. For the sake of completeness, Appendix C is devoted to a method based on primitive functions.

Our starting point is a Lagrangian graph (4) satisfying (5) and a diffeomorphism $\phi : \mathbb{T}^d \to \mathbb{T}^d$ satisfying (6). Notice that, if $S : \mathbb{T}^d \times \mathbb{R}^d \to \mathbb{R}$ is the primitive function of F, then

$$S_L(x) = S(x, \nabla_x L(x)) - L(\bar{x}(x, \nabla_x L(x)) + L(x) \text{ is constant} . \tag{7}$$

This is useful to check the computations. (For more information about this property, see [23, 24] and Appendix C.)

The first step in the normal form procedure is to send the Lagrangian graph to the zero-section and to reduce the dynamics on the torus to a rotation. This is made by using a vertical translation and a point transformation. The *vertical translation* τ_L generated by the function L is given by

$$\bar{x} = x \pmod 1 , \ \bar{y} = y + \nabla_x L(x) .$$

The *lift* of the diffeomorphism ϕ, also known as the point transformation $\hat{\phi}$, is given by

$$\bar{x} = \phi(x) \pmod 1 , \ \bar{y} = (\mathrm{D}\phi(x))^{-\top} y ,$$

where $^{-\top}$ means the transpose of the inverse of a matrix.

Henceforth, the first step is made by using the transformation $\tau_{L,\phi} = \tau_L \circ \hat{\phi}$. It is clear that $\bar{F} = \tau_{L,\phi}^{-1} \circ F \circ \tau_{L,\phi}$ is an exact symplectomorphism that fixes the zero-section, whose dynamics is given by the rotation (notice that, however, $\tau_{L,\phi}$ is not exact if $a \neq 0$, but $\bar{F}$ is). The primitive function of $\bar{F}$ is

$$\bar{S} = S \circ \tau_{L,\phi} - L \circ \bar{x} \circ \tau_{L,\phi} + L \circ \phi .$$

Remark: Notice that sending the Lagrangian graph to the zero-section is numerically very easy. In general, for tori that are not graphs, we had to adapt symplectic coordinates around the Lagrangian torus. A rigorous construction is given by a Weinstein's theorem [38]. $\triangleleft$

So, our new starting point is an exact symplectomorphism F, whose primitive function S satisfies $\mathrm{D}S(x,0) = 0$, and such that the dynamics on the zero section is a rotation by ω.

We look for a primitive symplectomorphism G, whose primitive function is T, such that $\bar{F} = G{\circ}F{\circ}G^{-1}$ is as simple as possible. In particular, in [24] was shown that, if we take $T = T_{\leq n}$ as a suitable Fourier-Taylor polynomial of degree $n \geq 2$, we can get that the primitive function of $\bar{F} = G{\circ}F{\circ}G^{-1}$ is $\bar{S}(x,y) = N_{\leq n}(y) + R_{>n}(x,y)$, where $N_{\leq n}(y)$ is a polynomial of degree n and the order (in the y variables) of $R_{>n}(x,y)$ is $n+1$ (we will write $R_{>n}(x,y) = O(y^{n+1})$).

Formally speaking, the equation that we have to solve is

$$T{\circ}F + S = N{\circ}G + T \ . \tag{8}$$

Notice that we have reduced an equation involving maps (the symplectomorphisms) to an equation involving functions (their primitive functions). This equation can be solved up to order $n \geq 2$ (but arbitrary, depending on the degree of differentiability of the symplectomorphism and the properties of ω). So, $\bar{F}$ is given by

$$\bar{x} = \omega + x + \nabla_y H_{\leq n}(y) + O(y^n) \pmod 1 \ , \ \bar{y} = y + O(y^{n+1}) \ ,$$

where $H_{\leq n}$ is a polynomial of degree n satisfying $y \cdot \nabla_y H_{\leq n}(y) - H(y) = N_{\leq n}(y)$. The coefficients of N are the coefficients of the normal form. The most relevant terms are the second order terms, that are given by a symmetric matrix B that is known as the *torsion* of the torus: $N_2(y) = \frac{1}{2} y^\top B y$. So, a torus is classified as a non-degenerate torus, definite positive torus, undefinite torus, etc., depending on the corresponding properties of the matrix B. Degenerate tori appear in non-twist maps [14].

Remark: Notice that we look for G as a whole, rather than a composition of simpler symplectomorphisms (in our case, primitive symplectomorphism with homogeneous primitive functions), as is quite usual in the computation of normal forms. Although composition of maps is an expensive procedure, from the computational point of view, the convenience of the first method is rather practical than numerical. If one writes the composition procedures in a very efficient way, the computational effort using both methods is similar. $\triangleleft$

The equation (8) can be solved order by order in y. That is to say, we compute the coefficients $T_2(x), T_3(x), \ldots, T_k(x) \ldots$ of the primitive function of G and the coefficients $N_2, N_3, \ldots, \ldots N_k, \ldots$ of the primitive function of the normal form. At the step k, we have already computed $T_{<k}(x,y)$ and $N_{<k}(y)$, and the terms $T_k(x)$ and N_k (that are symmetric

k-multilinear maps with respect to the y variables) are computed from the equation:

$$\begin{aligned}&(T_k(x) - T_k(x+\omega) + N_k)(y)^k = \\ &-(T_{<k}(x,y) - T_{<k}\circ F(x,y) - S(x,y) + N_{<k}\circ\pi_y\circ G_{<k}(x,y))_k \ ,\end{aligned} \tag{9}$$

where $\pi_y : \mathbb{T}^d \times \mathbb{R}^d$ is the y-projection. This is a small divisor equation so typical in KAM theory. N_k is fixed to match the averages of both sides in (9), and we fix the average of T_k equal to zero.

In the normal form algorithm, we have used the iteration (9) to solve (8). Notice that we obtain one term in the expansion of T (and N) at each step. In the case $d = 1$, the algorithm reads as follows.

Algorithm 2 *Let $S : \mathbb{T}\times\mathbb{R} \to \mathbb{R}$ be the primitive function of an exact symplectomorphism $F = (f^1, f^2) : \mathbb{T} \times \mathbb{R} \to \mathbb{T} \times \mathbb{R}$ that fixes the zero-section, and such that the motion of the points on the zero-section is a rotation by a Diophantine number ω. The corresponding Fourier-Taylor expansions (input) are*

$$S(x,y) = \sum_{k\geq 2} S_k(x) y^k$$

and

$$\bar{x} = \omega + x + \sum_{k\geq 1} f_k^1(x) y^k \ , \ \bar{y} = \sum_{k\geq 1} f_k^2(x) y^k \ .$$

The relation between the the coefficients $f_k^1(x)$ and $f_k^2(x)$ and S_k is given by Algorithm 1.

The output is given by the coefficients (to a fixed order) of the primitive function of the normal form

$$N(y) = \sum_{k\geq 2} N_k y^k \ ,$$

the change of variables $G = (g^1, g^2)$

$$\bar{x} = x + \sum_{k\geq 1} g_k^1(x) y^k \ , \ \bar{y} = \sum_{k\geq 1} g_k^2(x) y^k \ ,$$

where $g_1^2 = 1$, and its primitive function

$$T(x,y) = \sum_{k\geq 2} T_k(x) y^k \ .$$

In order to compute them at each step $k \geq 2$ we proceed as follows:

- *Compute*

$$C_k(x) = -(T_{<k}(x,y) - T_{<k}\circ F(x,y) - S(x,y) + N_{<k}\circ\pi_y\circ G_{<k}(x,y))_k \ ;$$

- *N_k is the average of the periodic function $C_k(x)$;*
- *Solve the small divisors equation*

$$T_k(x,y) - T_k(x+\omega) = C_k(x) - N_k \ ;$$

- *Compute the terms $g^1_{k-1}(x)$ and $g^2_k(x)$ of the expansion of G:*

$$g^1_{k-1}(x) = \frac{k}{k-1} T_k(x) - \frac{1}{k-1} \sum_{u=1}^{k-2} u g^1_u(x) g^2_{k-u}(x) \ ,$$
$$g^2_k(x) = T'_k(x) - {g^1_{k-1}}'(x) - \sum_{u=1}^{k-2} {g^1_u}'(x) g^2_{k-u}(x) \ .$$

5 Numerical implementation of the algorithms

We have implemented the algorithms in a computer, using C programming language. The computations have been carried out in a PC Pentium III, with a CPU of 731.484 MHz and a cache size of 256 Kb, working under Linux operative system. What follows is a report of some numerical results. The pictures have been made using `gnuplot` and `xmgrace`.

5.1 Generation of TLP symplectomorphisms

The total change of variables in the normal form procedure is a *TLP symplectomorphism*: a composition of a primitive symplectomorphism, a lift and a vertical translation. The object of this section is to illustrate the usefulness of TLP symplectomorphisms to generate dynamics.

A TLP symplectomorphism $F = T \circ L \circ P$ is a combination of different dynamical behaviours:

- P is a primitive symplectomorphism, and so it fixes all the points of the zero-section, and it is determined by its primitive function $S : \mathbb{T}^d \times \mathbb{R}^d \to \mathbb{R}$, that satisfies $\mathrm{D}S(x,0) = 0$;
- L is a lift of a diffeomorphism $\phi : \mathbb{T}^d \to \mathbb{T}^d$, and it moves the points on the zero-section;
- T is a vertical translation generated by the function $l(x) = a \cdot x + \bar{l}(x)$, where $a \in \mathbb{R}^d$ and $\bar{l} : \mathbb{T}^d \to \mathbb{R}$, and it sends the zero-section to a Lagrangian graph.

Notice that a TLP symplectomorphism F is characterized by that fact that the image of the zero-section is a Lagrangian graph $y = \frac{\partial l}{\partial x}(x)$. From this, TLP symplectomorphisms are useful to codify an open set of symplectomorphisms: those that send the zero-section to a Lagrangian graph.

Example: As an example, consider the family TLP where:

- P is the primitive symplectomorphism given by

$$S(x,y) = \frac{1}{2}(a + \frac{b}{2\pi}\sin(2\pi x))y^2 + \frac{1}{3}y^3 \ ;$$

- L is the lift of a rotation by $\omega \in \mathbb{R}$: $L(x,y) = (\omega + x, y)$;
- T is the vertical translation by $l'(x) = -\frac{\lambda}{2\pi}\sin(2\pi x)$: $T(x,y) = (x, y + l'(x))$.

We have used the Algorithm 1 to produce the primitive symplectomorphism P from its primitive function S up to order 50. Then, we have estimated a 'convergence' neighbourhood around $\{y = 0\}$ where the expansions of P are good enough.

By varying the parameters ω, λ, a, b we obtain different types of dynamics. Several examples are shown in Fig. 1 and Fig. 2. $\triangleleft$

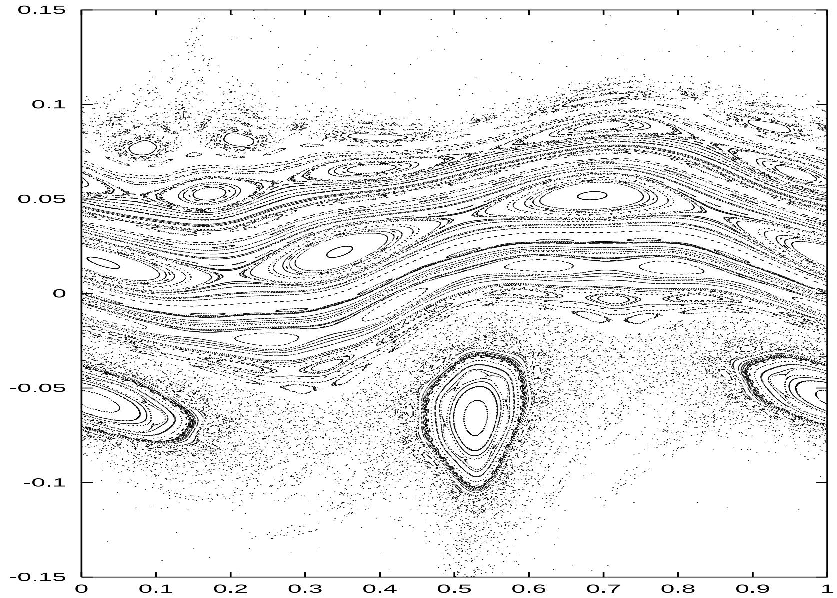


Figure 1: Dynamics of TLP in the case $\omega = \frac{\sqrt{5}-1}{2}, \lambda = .25, a = 2, b = 8$. This is an example of twist dynamics.

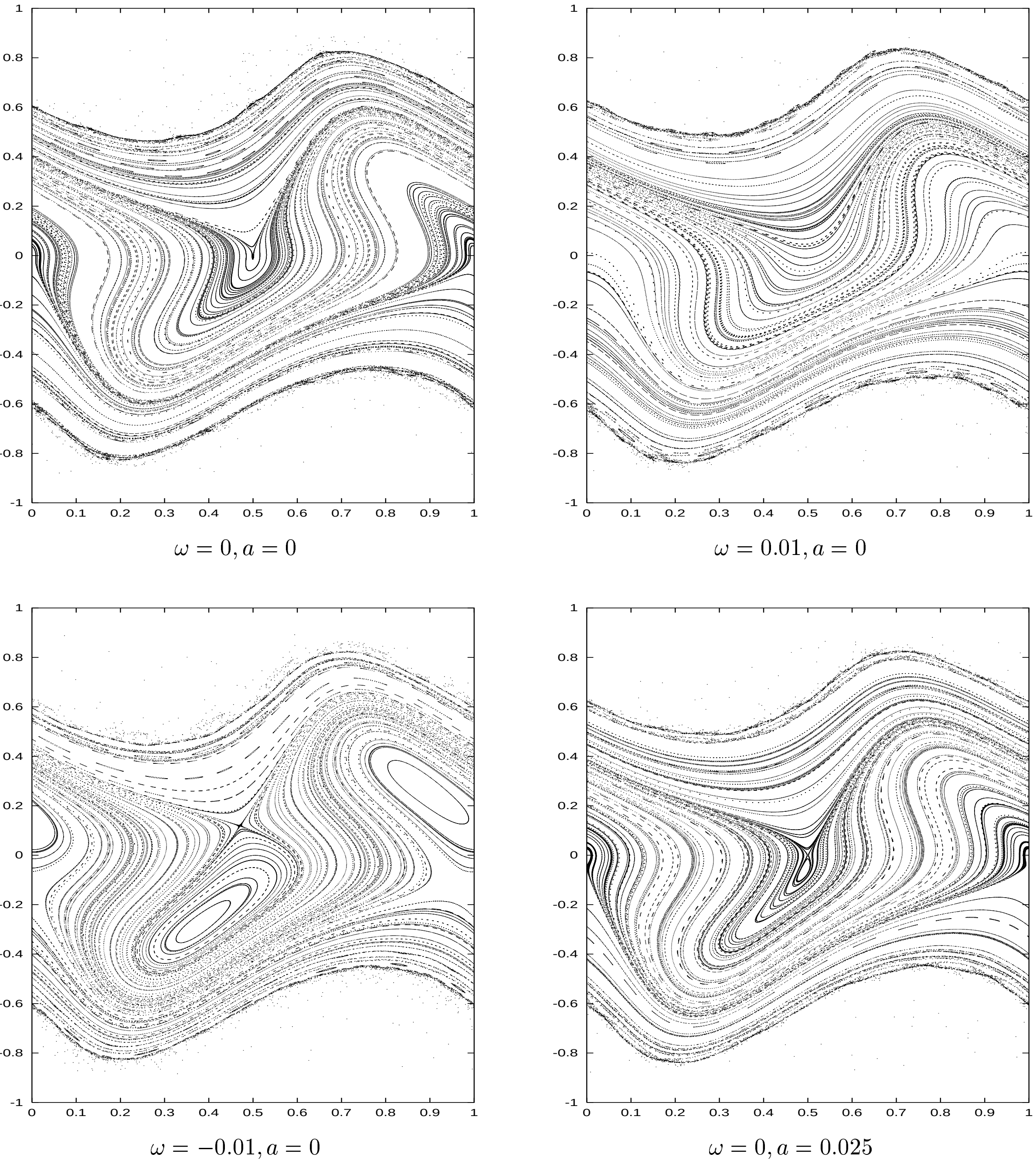


Figure 2: The values of the parameters of TLP are $\lambda = .25$ and $b = 1$, and both values of ω and a are near 0. Notice the existence of meandering invariant curves [12, 36, 23]. These are examples of non-twist dynamics.

5.2 Computation of the normal form of a rotational invariant curve

In this section we compute the normal form of a rotational invariant graph of an area preserving map. Two models have been considered: the standard map and the quadratic standard map.

Example: The *standard map* [13] is a map on the annulus $\mathbb{T} \times \mathbb{R}$ given by

$$\bar{x} = x + \bar{y} \pmod 1 \ , \ \bar{y} = y - \frac{K}{2\pi} \sin(2\pi x) \ .$$

K is a parameter that introduces non-integrability in the system (when $K = 0$, the system is integrable). It is know that the invariant torus corresponding to the golden mean $\omega = \frac{\sqrt{5}-1}{2}$ rotation vector does exist for $K = 0.93$ [33]. In fact, there is numerical evidence that such torus survives for values $K < 0.971635$ (see, for instance, [21, 29, 34]).

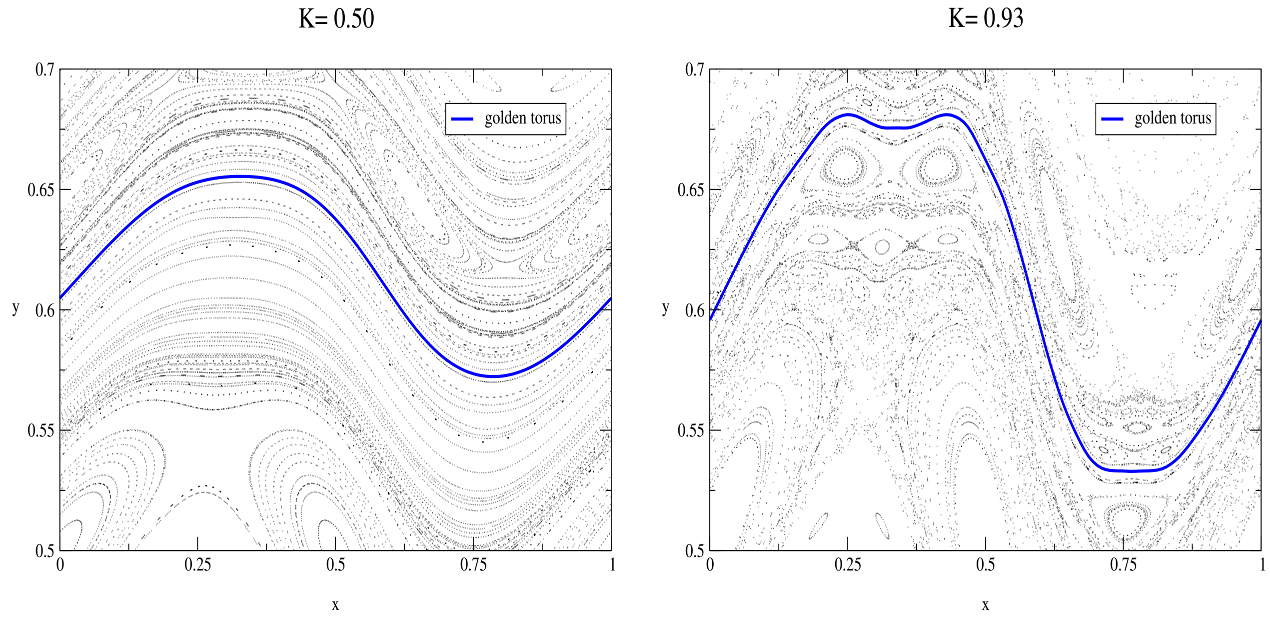
Fig. 3 shows the first coefficients of the normal form of the golden torus with frequency $\omega = \frac{1}{2}(\sqrt{5} - 1)$ for $K = 0.5$ and $K = 0.93$. We also estimate the errors and the execution time. $\triangleleft$

Example: The second example is a *quadratic standard map* on the annulus:

$$\bar{x} = \lambda + x + \bar{y}^2 \pmod 1 \ , \ \bar{y} = y - \frac{K}{2\pi} \sin(2\pi x).$$

In this case K introduces again non integrability in the system and λ gives a shift on the rotation numbers of the orbits. This map is non-twist: the twist is positive above the critical curve $y = \frac{K}{2\pi} \sin(2\pi x)$ and negative below such curve [23]. It is know that meandering phenomena as in Fig. 2 can appear for non-twist maps [12, 36, 23]. We will choose the parameters to avoid this case.

In Fig. 4 we see the disappearance of the pair of tori with frequency $\omega = \frac{1}{2}(3 - \sqrt{5})$. λ is fixed as 0.375, a rational number near (and below) ω. Notice that for $K = 0$, both tori exists in the levels $y = \pm\sqrt{\omega - \lambda}$, one has positive twist and the other one has negative twist. When increasing the parameter K, those tori cross the critical curve and approach each other. $\triangleleft$



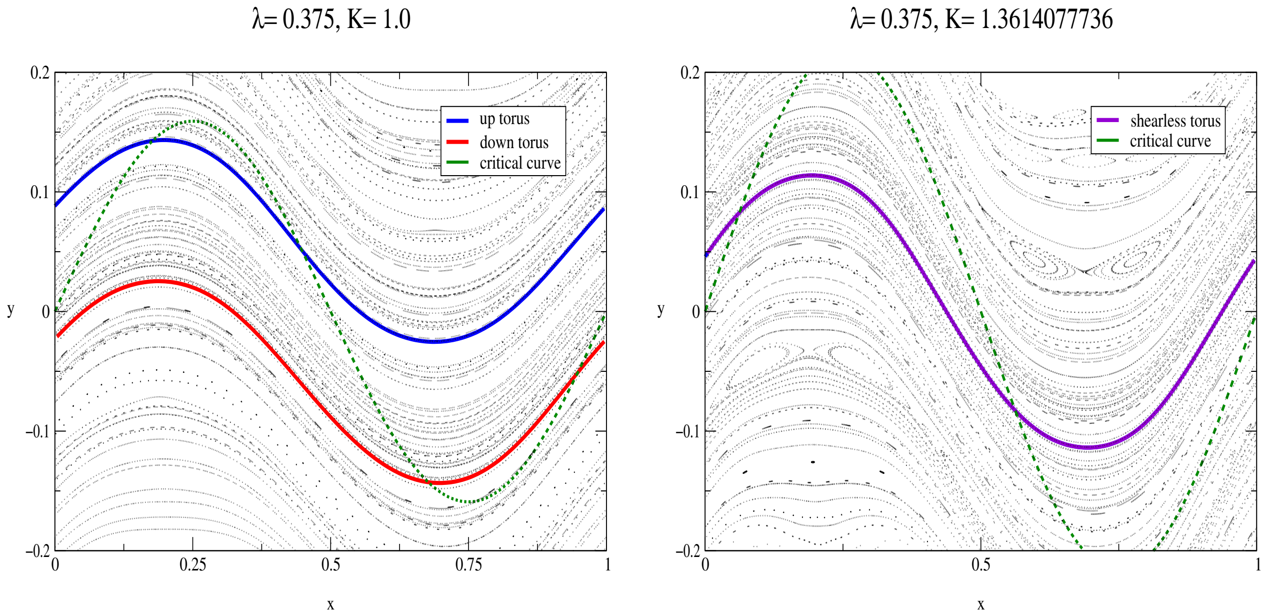
	Conserved quantity	Error
S_L	1.905250477570824e–01	1.3e–17

	Normal form coefficients	Error
N_0	0.000000000000000e+00	8.1e–19
N_1	0.000000000000000e+00	3.9e–17
N_2	5.074352766781860e–01	2.8e–17
N_3	3.498169925261595e–02	2.0e–15
N_4	1.264678937502437e+00	3.0e–13
N_5	4.276060590571166e+00	8.5e–11

	Conserved quantity	Error
S_L	1.893721014991033 7e–01	6.5e–13

	Normal form coefficients	Error
N_0	0.000000000000000e+00	1.4e–12
N_1	0.000000000000000e+00	1.5e–09
N_2	5.634607958050388e–01	8.3e–15
N_3	7.451666993207747e–01	1.2e–10
N_4	8.013735579646330e+04	4.2e–06
N_5	-4.526711981164502e+06	2.8e–01

Figure 3: **Golden torus for the standard map.** The pictures show the KAM tori with frequency $\omega = \frac{1}{2}(\sqrt{5}-1)$, for the values $K = 0.5$ and $K = 0.93$ of the standard map. Below each picture, two tables are presented: the first one shows the conserved quantity C, that is the average of $S_L(x)$ (see (7)), and an estimate of the error (the sup norm of $S_L(x) - C$); the second one shows the six first terms of the primitive function of the normal form, and estimates of the errors (the sup norms of the first six Taylor coefficients of $T{\circ}F + S - N{\circ}G - T$).
Notice that closer we are to the breakdown, bigger are the coefficients of the normal form. They explode in the breakdown.
(While we need 150 harmonics to expand the torus for $K = 0.5$, this number increases to 250 for $K = 0.93$. The execution times in the computation of the corresponding normal forms are $1m31.750s$ and $7m42.380s$, respectively.)



	Conserved quantity	Error
S_L	1.240170635035874e–04	7.8e–20

	Normal form coefficients	Error
N_0	0.000000000000000e+00	8.2e–20
N_1	0.000000000000000e+00	8.1e–21
N_2	5.617318688130254e–02	5.2e–18
N_3	6.531507200319253e–01	1.4e–17
N_4	5.191983218671878e–02	1.0e–17
N_5	2.391633538363182e–01	1.2e–15

	Conserved quantity	Error
S_L	9.700000000000000e–18	1.2e–10

	Normal form coefficients	Error
N_0	0.000000000000000e+00	1.1e–10
N_1	0.000000000000000e+00	1.7e–10
N_2	3.279562910144461e–09	7.0e–18
N_3	6.370957460790143e–01	1.3e–17
N_4	6.360110805374549e–09	7.9e–17
N_5	4.942121748139058e–01	4.8e–16

Figure 4: **Collision of two KAM tori in the quadratic standard map.** For $\lambda = 0.375$, $K = 1.0$, the quadratic standard map has two invariant tori (up and down) with frequency $\omega = \frac{1}{2}(3-\sqrt{5})$. Although these tori are non twist (they cross the critical curve), they are definite. The tables correspond to the up torus, and it is shown that N_2 is positive for $K = 1.0$. In suitable coordinates (given by the first step of the normal form procedure), the twist of the up torus is positive.
When the value of K is increased to $K \simeq 1.3614$, both tori merge in an unique degenerate torus: the shearless torus [11]. The most relevant coefficient of the normal form is, then, the third one, N_3. In suitable coordinates, the shearless torus separates the phase space in a positive twist region and a negative twist region. For $K > 1.3614$, there are not tori with rotation number ω.
(We just need 150 harmonics to expand all the tori in these pictures. The execution times in the computation of the normal forms are around $1m30s$.)

Conclusions and perspectives

In this paper we have presented the computation of normal forms around maximal invariant tori for symplectic diffeomorphisms, both twist and non-twist. The methods are based on the properties of the primitive function, and henceforth on the additional geometrical structure introduced by the action form. Not only these new algorithms let us to study degenerate situations, but also they provide faster methods to generate canonical transformations.

We have implemented numerically in this paper the simplest case in which the maximal invariant tori are 1D (and the phase space is 2D) and they are graphs. However, notice also that all the algorithms presented in this paper work in the higher dimensional case. The next step would be also the implementation of the computation of symplectic coordinates around an invariant tori, to study those cases in which the tori are not graphs.

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A A system of PDEs

In Section 3 we need some results about the system of PDE's

$$\mathrm{D}f(y)^\top y = F(y)\ ,\ f(0) = 0\ , \tag{10}$$

where $y = (y_1, \ldots, y_d)$ is a d-dimensional variable, $F : \mathbb{R}^d \to \mathbb{R}^d$ is a known function that satisfies $F(0) = 0$, and $f : \mathbb{R}^d \to \mathbb{R}^d$ is the unknown function. This section is devoted to the solution of such a problem.

For the sake of simplicity, we are going to suppose that the functions are C^∞ and defined in $\mathbb{R}^d$, but these conditions can be relaxed (C^r functions in star-shaped open sets, or consider real analytic functions).

In order to solve (10), we need some results on radial derivatives. The radial derivative of a function $h : \mathbb{R}^d \to \mathbb{R}$ is

$$\mathbf{R}h(y) = \mathrm{D}h(y)y\ . \tag{11}$$

We consider $\mathbf{R}$ as defined on the space of functions that map the point 0 to the value 0. Next proposition says that $\mathbf{R}$ is invertible.

Proposition 1 *Let $H : \mathbb{R}^d \to \mathbb{R}$ be a function with $H(0) = 0$. The only function $h : \mathbb{R}^d \to \mathbb{R}$ satisfying*

$$\mathrm{D}h(y)\ y = H(y)\ ,\ h(0) = 0\ , \tag{12}$$

is given by

$$h(y) = \int_0^1 \frac{1}{t} H(ty)\ dt\ .$$

We will write $h = \mathbf{R}^{-1}(H)$.

Proof: Checking that such a function h is a solution of (12) is straightforward. Let $\bar{h}$ another solution of (12). Then, the difference $\delta = h - \bar{h}$ satisfies the Euler equation

$$\mathrm{D}\delta(y)\ y = 0\ ,$$

an so the function is constant (because the only homogeneous functions of order 0 that are regular in the origin are the constants). Since $\delta(0) = 0$, we are done with the proof of the proposition. □

We can extend the definition of the radial derivative to the space of maps $f : \mathbb{R}^d \to \mathbb{R}^d$, with 0 as a fixed point, by defining the radial derivative of a vector function as the vector of radial derivatives.

The equation (10) involves the operator $\mathbf{L}$ defined by

$$\mathbf{L}f(y) = (\mathrm{D}f(y))^\top y\ . \tag{13}$$

This equation is written in components as

$$\sum_{i=1}^d y_i \frac{\partial f_i}{\partial y_j}(y) = F_j(y)\ ,\ j = 1, \ldots, d\ . \tag{14}$$

We will write $\sum_i$ instead of $\sum_{i=1}^d$. Hence, for any $k = 1, \ldots, d$:

$$\begin{aligned}
\sum_j y_j \frac{\partial F_j}{\partial y_k} &= \sum_{i,j} y_i y_j \frac{\partial^2 f_i}{\partial y_j \partial y_k} + \sum_j y_j \frac{\partial f_k}{\partial y_j} \\
&= \sum_i y_i \mathbf{R}\left(\frac{\partial f_i}{\partial y_k}\right) + \mathbf{R}f_k \\
&= \sum_i \left(\mathbf{R}\left(y_i \frac{\partial f_i}{\partial y_k}\right) - y_i \frac{\partial f_i}{\partial y_k}\right) + \mathbf{R}f_k\ .
\end{aligned}$$

From here, we obtain that

$$f_k = \mathbf{R}^{-1}\left(\sum_j y_j \frac{\partial F_j}{\partial y_k} + F_k\right) - F_k \ , \tag{15}$$

and we will write $f = \mathbf{R}^{-1}\left(\mathrm{D}F(y)^\top y + F\right) - F$.

We summarize the previous explanation in the following proposition.

Proposition 2 *Let $F : \mathbb{R}^d \to \mathbb{R}^d$ be a vector function with $F(0) = 0$. The only vector function $f : \mathbb{R}^d \to \mathbb{R}^d$ satisfying*

$$\mathrm{D}f(y)^\top \ y = F(y) \ , \ f(0) = 0 \ ,$$

is given by

$$f(y) = \mathbf{R}^{-1}\left(\mathrm{D}F(y)^\top y + F\right)(y) - F(y) \ . \tag{16}$$

We will write $f = \mathbf{L}^{-1}F$.

B The classical methods

In this appendix, we are going to review some of the classical methods to generate exact symplectomorphisms. We will compare this methods with the one proposed in this paper.

For the sake of simplicity, the phase space will be $\mathbb{T}\times\mathbb{R}$. This is the case that we have implemented for the primitive function algorithm.

B.1 A generating function method

There are several ways of representing an exact symplectomorphism by means of generating functions. Here, we are going to consider one of them.

Let $F : \mathbb{T}\times\mathbb{R} \to \mathbb{T}\times\mathbb{R}$ be an exact symplectomorphism, denoted by

$$\bar{x} = x + f(x, y) \ , \bar{y} = g(x, y) \ ,$$

where $S : \mathbb{T}\times\mathbb{R} \to \mathbb{R}$ is its primitive function, i.e., S satisfies the exactness equations

$$\frac{\partial S}{\partial x} = \bar{y}\frac{\partial \bar{x}}{\partial x} - y \quad , \quad \frac{\partial S}{\partial y} = \bar{y}\frac{\partial \bar{x}}{\partial y} \ . \tag{17}$$

Suppose that for each $x \in \mathbb{T}$, $\bar{y}(x, \cdot) : \mathbb{R} \to \mathbb{R}$ is a diffeomorphism and let $\psi(x, \cdot) : \mathbb{R} \to \mathbb{R}$ be its inverse function: $\bar{y} = g(x, \psi(x, \bar{y}))$. So, by defining

$$H(x, \bar{y}) = x\bar{y} + \bar{y}\cdot f(x, \psi(x, \bar{y})) - S(x, \psi(x, \bar{y})) \ ,$$

we obtain the relations

$$\bar{x} = \frac{\partial H}{\partial \bar{y}}(x, \bar{y}) \quad , \quad y = \frac{\partial H}{\partial x}(x, \bar{y}) \ , \tag{18}$$

that determine implicitly the symplectomorphism F.

If F is a primitive symplectomorphism, the Fourier-Taylor expansion of the generating function H is like

$$H(x, \bar{y}) = x\bar{y} + \sum_{n \geq 2} h_n(x)\bar{y}^n. \tag{19}$$

The coefficients $h_n(x)$ $(n \geq 2)$ are periodic functions (given by Fourier series). We denote $h(x, \bar{y}) = \sum_{n \geq 2} h_n(x)\bar{y}^n$.

We want to recover F from the relations (18). The first functional equation that we have to solve is

$$y = g(x, y) + \frac{\partial h}{\partial x}(x, g(x, y)) \ ,$$

from where we obtain g.

This explanation leads to the following algorithm.

Algorithm 3 *Let $h : \mathbb{T} \times \mathbb{R} \to \mathbb{R}$ be a function whose Fourier-Taylor expansion is*

$$h(x, \bar{y}) = \sum_{n \geq 2} h_n(x)\bar{y}^n \quad \text{(input)}.$$

The symplectomorphism F whose generating function is $H(x, \bar{y}) = x\bar{y} + h(x, \bar{y})$ is a primitive symplectomorphism expanded by

$$\bar{x} = x + \sum_{n \geq 1} f_n(x)y^n \ , \ \bar{y} = \sum_{n \geq 1} g_n(x)y^n \qquad \text{(output)},$$

where the coefficients $g_n(x)$ are computed by the recurrence

$$\begin{aligned} &\textit{step 1:} \qquad && g_1(x) = 1 \ ; \\ &\textit{step n:} \qquad && g_n(x)y^n = y - \sum_{k=2}^{n} h_k{}'(x)(g_{<n}(x, y))^k \mod y^{n+1} \ , \end{aligned}$$

where mod y^{n+1} *means that we neglect all the terms of order bigger than n. The expansion of $\bar{x}$ is recovered from*

$$f(x, y) = \frac{\partial h}{\partial \bar{y}}(x, g(x, y)) \ .$$

If we are given $H_{\leq N}(x, y)$, we can compute $g_{\leq N}(x, y)$, and we compute $f_{<N}(x, y)$ by

$$f_{<N}(x, y) \quad = \quad x + \sum_{k=1}^{N-1} (k+1)h_{k+1}(x)(g_{\leq N}(x, y))^k \mod y^N \ .$$

Number of Fourier products. Notice that the number of products of Fourier series in the step n of the computation of g_n is $O(\frac{1}{2}n^2)$. We have to compute the n first powers of $g_n(x,y)$, but we already know from the previous step the $n-1$ first powers of $g_{n-1}(x,y)$. Hence, to reach the order N in the computation of g, we have to do $O(\frac{1}{6}N^3)$ products of Fourier series. The computation of f up to order $N-1$ carries also about $O(\frac{1}{6}N^3)$ products. So, the total number of products is $O(\frac{1}{3}N^3)$.

B.2 The Lie transform method

A time-independent Hamiltonian, $H = H(x,y)$, generates an exact symplectic flow φ_t. In particular, the time-1 map $F = \varphi_1$ is an exact symplectomorphism. Notice that in the 2-dimensional case that we are considering here, we are generating an integrable map because it has a conserved quantity, H.

The Lie transform provides a method to compute the composition $p\circ\varphi_t$, where $p = p(x,y)$ is an arbitrary function (in particular, we are interested in the cases $p(x,y) = x$ and $p(x,y) = y$). This method is based on the well-known formula

$$p\circ\varphi_t = \sum_{k\geq 0} \frac{t^k}{k!} L_H^k p \ , \tag{20}$$

where $L_H^0 p = p$ and $L_H^{k+1} p = \{H, L_H^k p\}$. Here, $\{\cdot,\cdot\}$ is the Poisson bracket

$$\{H_1, H_2\} = \frac{\partial H_1}{\partial y}\frac{\partial H_2}{\partial x} - \frac{\partial H_1}{\partial x}\frac{\partial H_2}{\partial y} \ .$$

If the Hamiltonian H is like

$$H(x,y) = \sum_{n\geq 2} h_n(x) y_n \ ,$$

then F is a primitive symplectomorphism. By defining $\bar{x} = \pi_x\circ\varphi_1$, $\bar{y} = \pi_y\circ\varphi_1$ and using the formula (20), we can compute the expansions of F. Suppose that we are given H to order N. Then we can compute $\bar{x}$ to order $N-1$ and $\bar{y}$ to order N.

Algorithm 4 *Let $H : \mathbb{T}\times\mathbb{R}\to\mathbb{R}$ be a function whose Fourier-Taylor expansion is*

$$H(x,y) = \sum_{n\geq 2} h_n(x) y^n \quad \text{(input)}.$$

The symplectomorphism F given by the time-1 map φ_1 of the Hamiltonian vector field generated by H is a primitive symplectomorphism that can be expanded by

$$\bar{x} = \sum_{k\geq 0} \frac{1}{k!} f_k(x,y) \ , \ \bar{y} = \sum_{k\geq 0} \frac{1}{k!} g_k(x,y) \quad \text{(output)},$$

where the functions $f_k(x,y)$ and $g_k(x,y)$ can be computed by means of the recurrence

$$\begin{array}{ll} \textit{step } 0: & f_0(x,y) = x \ , \ g_0(x,y) = y \ ; \\ \textit{step } k: & f_k(x,y) = \{H, f_{k-1}\} \ , \ g_k(x,y) = \{H, g_{k-1}\} \ . \end{array}$$

If we know $H_{\leq N}(x,y)$, we can compute $f_{<N}(x,y)$ and $g_{\leq N}(x,y)$. To do so, we have to perform N steps of the algorithm, and to do the f-calculations mod y^N *and the g-calculations* mod y^{N+1}.

Number of Fourier products. Notice that $f_k(x,y)$ begins with terms of order k in y, that is, $f_k(x,y) = y^k \hat{f}_k(x,y)$ for a suitable $\hat{f}$. Similarly, $g_k(x,y) = y^{k+1}\hat{g}_k(x,y)$. So, the computation of each Poisson bracket in the k term of the expansion needs $(N-n)(N-n+1)$ products of Fourier series. So then, the total number of products of Fourier series to reach the order N is $O(\frac{2}{3}N^3)$.

Remark: The algorithms that we have considered here using the generating function method and the Lie transform method are not the more effective, but the simpler. Like in the primitive function algorithm, we compute just one homogeneus term at each step of the procedure.

There are several ways to improve the algorithms. For instance, in the case of the generating function method we can use Newton's method to solve the implicit equation to get a quadratic algorithm, in the sense that doing k steps of the procedure we get 2^k terms of the expansions. In the Lie transform method, we can use FFT-based techniques to perform the operations with Taylor polynomials (see, for instance [1]). In both cases, the number of Fourier products can be gone down to $O(N^2 \log N)$, still far from $O(N^2)$.

A curious fact is that using Newton's method to solve the exactness equation (2) of the primitive function method the number of Fourier products is again $O(N^2)$.

We point out that these numbers correspond to the case $d = 1$, and the differences among the methods will be much bigger in higher dimensions. $\triangleleft$

C Primitive function and invariant Lagrangian graphs

In this section we explain some properties of invariant Lagrangian graphs, which can be used as the basis of an algorithm to compute invariant KAM tori that are graphs [15].

Proposition 3 *Let $F : \mathbb{T}^d \times \mathbb{R}^d \to \mathbb{T}^d \times \mathbb{R}^d$ be an exact symplectomorphism, where $S : \mathbb{T}^d \times \mathbb{R}^d \to \mathbb{R}$ is its primitive function. Let*

$$y = a + \nabla_x l(x) \ , \tag{21}$$

a Lagrangian graph generated by the function $L(x) = a \cdot x + l(x)$, where $a \in \mathbb{R}^d$ and $l : \mathbb{T}^d \to \mathbb{R}$. Suppose that the map $\bar{x}_L : \mathbb{T}^d \to \mathbb{T}^d$ defined by

$$\bar{x}_L(x) = \bar{x}(x, \nabla_x L(x))$$

is a diffeomorphism, and define the function $S_L : \mathbb{T}^d \to \mathbb{R}$ *by*

$$S_L(x) = S(x, \nabla_x L(x)) - L(\bar{x}_L(x)) + L(x) \ .$$

Then:

The Lagrangian graph (21) is F*-invariant* $\Leftrightarrow$ $S_L(x)$ *is constant.*

The proof is straightforward (cf. [23]). As a corollary, we characterise KAM tori.

Proposition 4 *Let* $F : \mathbb{T}^d \times \mathbb{R}^d \to \mathbb{T}^d \times \mathbb{R}^d$ *be an exact symplectomorphism, where* $S : \mathbb{T}^d \times \mathbb{R}^d \to \mathbb{R}$ *is its primitive function. Then, a KAM torus (graph) of frequency vector* $\omega \in \mathbb{R}^d$ *is characterised by a generating function* $L(x) = a \cdot x + l(x)$*, a constant* C *and a diffeomorphism* $\phi : \mathbb{T}^d \to \mathbb{T}^d$ *satisfying the relations*

$$\begin{aligned} & S(x, \nabla_x L(x)) - L(\bar{x}_L(x)) + L(x) = C \ , \\ & \bar{x}_L(\phi(\theta)) = \phi(\theta + \omega) \ , \end{aligned} \tag{22}$$

where $\bar{x}_L(x) = \bar{x}(x, \nabla_x L(x))$*.*

The previous proposition characterises KAM tori that are graphs. Given a graph that is approximately invariant, and an approximate conjugation to the rotation ω, we can apply Newton method to improve the error estimates. The following lines are highly inspired in [28].

Suppose that we are given a Lagrangian graph generated by $L(x) = a \cdot x + l(x)$ and a diffeomorphism on the torus $\phi(\theta) = \theta + \varphi(\theta)$ such that

$$S(x(\theta), y(\theta)) - L(x(\theta + \omega)) + L(\theta) = E(\theta) \ , \tag{23}$$

$$\bar{x}(x(\theta), y(\theta)) - x(\theta + \omega) = e(\theta) \ , \tag{24}$$

where $x(\theta) = \phi(\theta)$ and $y(\theta) = \nabla_x L(\phi(\theta))$, and the errors $E(\theta) - \bar{E}$ (and their derivatives) and $e(\theta)$ are small. ($\bar{E}$ is the average of $E(\theta)$.)

We would like to produce better $L(x)$ and $\phi(\theta)$. So, let $\Delta L(x) = \Delta a \cdot x + \Delta l(x)$ and $\Delta\phi(\theta)$ the corresponding improvements. That is, we want that $L(x) + \Delta L(x)$ and $\phi(\theta) + \Delta\phi(\theta)$ give smaller errors in (22) (in fact, quadratically small with respect to the previous ones). In the following, we are going to neglect quadratically small terms.

Firstly, from

$$\begin{aligned} C &= S(x, \nabla_x L(x)) + \nabla_x \Delta L(x)) \\ &\quad - (L(\bar{x}(x, \nabla_x L(x) + \nabla_x \Delta L(x))) + \Delta L(\bar{x}(x, \nabla_x L(x) + \nabla_x \Delta L(x)))) \\ &\quad + L(x) + \Delta L(x) \\ &= E \circ \phi^{-1}(x) + \bar{y}(x, \nabla_x L(x))^\top \frac{\partial \bar{x}}{\partial x}(x, \nabla_x L(x)) \nabla_x \Delta L(x) \\ &\quad - \frac{\partial L}{\partial x}(\bar{x}(x, \nabla_x L(x))) \nabla_x \Delta L(x) - \Delta L(\bar{x}(x, \nabla_x L(x))) + \Delta L(x) \\ &= E \circ \phi^{-1}(x) - \Delta L(\bar{x}_L(x)) + \Delta L(x) \ , \end{aligned}$$

then

$$\begin{aligned} E(\theta) - C &= \Delta L(\phi(\theta+\omega)) - \Delta L(\phi(\theta)) \\ &= \omega \cdot \Delta a + \Delta a \cdot (\varphi(\theta+\omega) - \varphi(\theta)) + \Delta l(\phi(\theta+\omega)) - \Delta l(\phi(\theta)) \ . \end{aligned}$$

So, by defining $\Delta l(\phi(\theta)) = -\Delta a \cdot \varphi(\theta) + H(\theta)$, we look for a periodic function $H(\theta)$ satisfying the equation

$$H(\theta+\omega) - H(\theta) = E(\theta) - \omega \cdot \Delta a - C \ . \tag{25}$$

Δa will be chosen later, and we will chose C in such a way the right part of (25) has average equal to zero. (25) is an small divisor equation, that can be solved when ω is Diophantine.

Denote $A(\theta) = \frac{\partial \bar{x}}{\partial x}(x(\theta), y(\theta))$ and $B(\theta) = \frac{\partial \bar{x}}{\partial y}(x(\theta), y(\theta))$. The conjugation property reaches

$$\begin{aligned} 0 &= \bar{x}(x(\theta) + \Delta x(\theta), y(\theta) + \Delta y(\theta)) - x(\theta+\omega) - \Delta x(\theta+\omega) \\ &= e(\theta) + A(\theta)\Delta\phi(\theta) + B(\theta)\left(\mathrm{D}^2 L(\phi(\theta))\Delta\phi(\theta) + \nabla_x \Delta L(\phi(\theta))\right) \\ &\quad -\Delta\phi(\theta+\omega) \\ &= e(\theta) + \mathrm{D}\phi(\theta+\omega)\mathrm{D}\phi(\theta)^{-1}\Delta\phi(\theta) + B(\theta)\mathrm{D}\phi(\theta)^{-\top}(\Delta a + \nabla_\theta H(\theta)) \\ &\quad -\Delta\phi(\theta+\omega) \ , \end{aligned}$$

where we neglect again all the quadratically small terms. By defining $\Delta\phi(\theta) = \mathrm{D}\phi(\theta)h(\theta)$, we obtain the equation

$$\begin{aligned} &h(\theta+\omega) - h(\theta) = \\ &\quad \mathrm{D}\phi(\theta+\omega)^{-1}\left(e(\theta) + B(\theta)\mathrm{D}\phi(\theta)^{-\top}(\Delta a + \nabla_\theta H(\theta))\right) \ , \end{aligned} \tag{26}$$

where we fix Δa to cancel the average in the right term and solve for h.

Notice that we can compute Δa if the average of

$$\mathrm{D}x(\theta+\omega)^{-1} B(\theta) \mathrm{D}x(\theta)^{-\top}$$

is a regular matrix. This is related with the fact that the torsion of the torus is non degenerate.

D A final digression on primitive functions

It is a remarkable fact that the primitive function of an exact symplectomorphism F on an exact symplectic manifold $(M, \omega = \mathrm{d}\alpha)$ is not a symplectically invariant object associated to F: it depends on the extra geometric properties of phase space given by the election of an action form α.

This could be an annoying fact [5], but we can make the most of it by adapting the geometry (the action form) to the problem that we are interested in.

In this paper we have been interested in the dynamics around KAM tori that are graphs. The phase space is $\mathbb{T}^d \times \mathbb{R}^d$ and the symplectic form is $\omega = dy \wedge dx$. The election of the action form $\alpha = y\ dx$ is not accidental: α vanishes on the zero-section, and it has associated a Lagrangian foliation whose leaves, the vertical leaves $x = x_0$, are transversal to the Lagrangian graph. Once we have pushed the Lagrangian graph on the zero-section, the use of the so called primitive symplectomorphisms makes the computation of normal forms a lot easier, because these symplectomorphisms are specially adapted to the action form $\alpha = y\ dx$.

Let us see another example. Suppose that we were interested in the local study of a fixed point of a symplectomorphism on the plane $\mathbb{R} \times \mathbb{R}$, where the canonical symplectic form is $\omega = dy \wedge dx$ (most of what follows also works in $\mathbb{R}^d \times \mathbb{R}^d$). Once we have moved the fixed point to the origin, it is quite standard to use symplectic changes of variables that are near to the identity to construct normal forms. Such a symplectomorphism F is given by

$$\bar{x} = x + f(x,y)\ ,\ \bar{y} = y + g(x,y)\ , \tag{27}$$

where f and g are $O(2)$ in x, y. There are many ways of generating near to the identity symplectomorphisms, the question for us is how to produce them using primitive functions (and to get faster methods). The first step is to choose a suitable action form. In this case we take $\alpha = \frac{1}{2}(ydx - xdy)$, because it vanishes on the origin. The corresponding exactness equations are

$$2\frac{\partial S}{\partial x} = \bar{y}\frac{\partial \bar{x}}{\partial x} - \bar{x}\frac{\partial \bar{y}}{\partial x} - y\ ,\ 2\frac{\partial S}{\partial y} = \bar{y}\frac{\partial \bar{x}}{\partial y} - \bar{x}\frac{\partial \bar{y}}{\partial y} + x\ . \tag{28}$$

S is the primitive function of F with respect to the above action form. As F is given by (27), $S = O(3)$. As in Section 3, we can write a fixed point equation for f and g (from where we can obtain the recurrences that expand f and g):

$$\begin{aligned} f &= \mathbf{E}\left(-2\frac{\partial S}{\partial y} - x\left(\frac{\partial f}{\partial x} + \frac{\partial g}{\partial y}\right) + g\frac{\partial f}{\partial y} - f\frac{\partial g}{\partial y}\right)\ , \\ g &= \mathbf{E}\left(+2\frac{\partial S}{\partial x} - y\left(\frac{\partial f}{\partial x} + \frac{\partial g}{\partial y}\right) - g\frac{\partial f}{\partial x} + f\frac{\partial g}{\partial x}\right)\ , \end{aligned} \tag{29}$$

where $\mathbf{E}$ is the linear operator on the space of functions of order 2 in the origin defined by

$$\mathbf{E}h(x,y) = -\int_0^1 \frac{1}{t^2} h(tx,ty)dt\ .$$

Notice also that it is very useful to expand f and g in homogeneous polynomials

$$f(x,y) = \sum_{k\geq 2} f_k(x,y)\ ,\ g(x,y) = \sum_{k\geq 2} g_k(x,y)\ ,$$

and that the operator $\mathbf{E}$ fixes the homogeneous levels: $\mathbf{E}h_k = \frac{-1}{k-1}h_k$ for a homogeneous polynomial of degree $k > 1$. Obtaining the recurrences for f_k and g_k is then straightforward.

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